A note on efficient computation of hybridization number via softwired clusters

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Abstract. Here we present a new fixed parameter tractable algorithm to compute the hybridization number $r$ of two rooted binary phylogenetic trees on taxon set $X$ in time $(6r)^r \cdot poly(n)$, where $n = |X|$. The novelty of this approach is that it avoids the use of Maximum Acyclic Agreement Forests (MAAFs) and instead exploits the equivalence of the problem with a related problem from the softwired clusters literature. This offers an alternative perspective on the underlying combinatorial structure of the hybridization number problem.

1 Introduction

For notation and background we refer the reader to [2,1]. Let $T_1$ and $T_2$ be the set of clusters obtained from two trees $T$ we can further restrict our attention to binary networks.

Observation 1. Let $C$ be an ST-collapsed set of clusters on $X$ such that $r(C) \geq 1$. Then the relation $\rightarrow_C$ is a partial order on $X$, the terminals are the maximal elements of the partial order and there is at least one terminal.

1 Note that, if a taxon $x$ appears in only one cluster, $\{x\}$, then (vacuously) $x \rightarrow_C y$ for all $y \neq x$.
Proof. The relation $\rightarrow_C$ is clearly reflexive and transitive. To see that it is anti-symmetric, suppose there exist two elements $x \neq y \in \mathcal{X}$ such that $x \rightarrow_C y$ and $y \rightarrow_C x$. Then we have that, for every non-singleton cluster $C \in \mathcal{C}$, $C \cap \{x, y\}$ is either equal to $\emptyset$ or $\{x, y\}$ i.e. $C$ is compatible with $\{x, y\}$. Furthermore, the only clusters that can possibly be in $\mathcal{C}(\{x, y\})$ are $\{x\}, \{y\}$ and $\{x, y\}$ and these are all mutually compatible. So $\{x, y\}$ is an ST-set, contradicting the fact that $C$ is ST-collapsed. Hence $\rightarrow_C$ is a partial order. The fact that the terminals are the maximal elements of the partial order then follows immediately from their definition. Finally, it is well known that every partial order on a finite set of elements contains at least one maximal element (because otherwise a cycle exists which contradicts the anti-symmetry property).

Let $T$ be a phylogenetic tree on $\mathcal{X}$. For a vertex $u$ of $T$ we define $\mathcal{X}(u) \subseteq \mathcal{X}$ to be the set of all taxa that can be reached from $u$ by directed paths. For a taxon $x \in \mathcal{X}$ we define $W^T(x)$, the witness set for $x$ in $T$, as $\mathcal{X}(u) \setminus \{x\}$, where $u$ is the parent of $x$. A critical property of $W^T(x)$ is that, for any non-singleton cluster $C \in \text{Cl}(T)$ that contains $x$, $W^T(x) \subseteq C$.\[\square\]

**Observation 2.** Let $\mathcal{C} = \text{Cl}(T)$ be a set of clusters on $\mathcal{X}$, where $T = \{T_1, T_2\}$ is a set of two binary trees on $\mathcal{X}$ with no non-trivial common subtrees, and $r(\mathcal{C}) \geq 1$. Then for any $x \in \mathcal{X}$ the following statements are equivalent: (1) $x$ is a terminal of $\mathcal{C}$; (2) there exist incompatible clusters $C_1, C_2 \in \mathcal{C}$ such that $C_1 \cap C_2 = \{x\}$; (3) $W^{T_1}(x) \cap W^{T_2}(x) = \emptyset$.

**Proof.** We first prove that (2) implies (1). For $x' \notin C_1 \cup C_2$ it holds that $x \not\rightarrow_C x'$, because $x \in C_1$ but $x' \notin C_1$. For $x' \in C_1 \setminus C_2$ it cannot hold that $x \rightarrow_C x'$, because $x \in C_2$ but $x' \notin C_2$, and this holds symmetrically for $x' \in C_2 \setminus C_1$. Hence $x$ is a terminal. We now show that (1) implies (3). Suppose (3) does not hold. Then there exists some taxon $x' \in W^{T_1}(x) \cap W^{T_2}(x)$. So every non-singleton cluster in $\mathcal{C}$ that contains $x$ also contains $x'$, irrespective of whether the cluster came from $T_1$ or $T_2$. But then $x \not\rightarrow_C x'$, so (1) does not hold. Hence (1) implies (3). Finally, we show that (3) implies (2). Note that (3) implies that in both $T_1$ and $T_2$ the parent of $x$ is not the root. If this was not so, then (wlog) $W^{T_1}(x) = \mathcal{X} \setminus \{x\}$, and combining this with the fact that $W^{T_1}(x), W^{T_2}(x) \neq \emptyset$ would contradict (3). Hence $W^{T_1}(x) \cup \{x\} \in \text{Cl}(T_1)$ and $W^{T_2}(x) \cup \{x\} \in \text{Cl}(T_2)$, from which (2) follows.\[\square\]

**Observation 3.** Let $\mathcal{C} = \text{Cl}(T)$ be a set of clusters on $\mathcal{X}$, where $T = \{T_1, T_2\}$ is a set of two binary trees on $\mathcal{X}$ with no non-trivial common subtrees, and $r(\mathcal{C}) \geq 1$. Then, for any two taxa $x \neq y \in \mathcal{X}$, $x \rightarrow_C y$ if and only if $y \in W^{T_1}(x) \cap W^{T_2}(x)$.

**Proof.** Suppose $x \rightarrow_C y$, but (wlog) $y \notin W^{T_1}(x)$. The parent of $x$ in $T_1$ cannot be the root, because then $W^{T_1}(x) = \mathcal{X} \setminus \{x\}$ which contains $y$. So there is an edge in $T_1$ whose head is the parent of $x$. Let $C \in \mathcal{C}$ be the cluster represented by this edge, then $C = \{x\} \cup W^{T_1}(x)$, $W^{T_1}(x)$ is non-empty and contains neither $x$ nor $y$, so $C$ is a non-singleton cluster which contains $x$ but not $y$. So $x \not\rightarrow_C y$. In the other direction, suppose $y \in W^{T_1}(x) \cap W^{T_2}(x)$. Let $C \in \mathcal{C}$ be a non-singleton cluster that contains $x$. Every non-singleton cluster $C \in \mathcal{C}$ is from $\text{Cl}(T_1)$ or $\text{Cl}(T_2)$, so $W^{T_1}(x) \subseteq C$ or $W^{T_2}(x) \subseteq C$. In any case it follows that $y \in C$.\[\square\]

**Lemma 1.** Let $\mathcal{C} = \text{Cl}(T)$ be a set of clusters on $\mathcal{X}$, where $T = \{T_1, T_2\}$ is a set of two binary trees on $\mathcal{X}$ with no non-trivial common subtrees, and $r(\mathcal{C}) \geq 1$. Let $x$ be any taxon in $\mathcal{C}$. If $x$ is not a terminal of $\mathcal{C}$ then there exists a terminal $y$ such that $x \rightarrow_C y$.

**Proof.** $\mathcal{C}$ is ST-collapsed because $T_1$ and $T_2$ contain no non-trivial common subtrees. Hence, by Observation 4 we know that $\rightarrow_C$ is a partial order on $\mathcal{X}$ and the terminals, of which there is at least one, are the maximal elements of the partial order. The result then follows immediately from the transitivity and anti-symmetry property of partial orders.\[\square\]

**Lemma 2.** Let $\mathcal{C} = \text{Cl}(T)$ be a set of clusters on $\mathcal{X}$, where $T = \{T_1, T_2\}$ is a set of two binary trees on $\mathcal{X}$ with no non-trivial common subtrees, and $r(\mathcal{C}) \geq 1$. Then there exists $x \in \mathcal{X}$ such that $r(\mathcal{C} \setminus \{x\}) < r(\mathcal{C})$.\[\square\]
Proof. Consider a binary network $N$ which represents $C$, where $r(N) = r(C)$. By acyclicity $N$ contains at least one Subtree Below a Reticulation (SBR) \cite{2}, i.e. a node $u$ with indegree-1 whose parent is a reticulation, and such that no reticulation can be reached by a directed path from $u$. Let $\mathcal{X}'$ be the set of taxa reachable from $u$ by directed paths. $\mathcal{X}'$ is an ST-set, so $|\mathcal{X}'| = 1$ (because $C$ is ST-collapsed). Let $x$ be the single taxon in $\mathcal{X}'$. Deleting $x$ and its reticulation parent from $N$ (and tidying up the resulting network in the usual fashion) creates a network $N'$ on $\mathcal{X}' \setminus \{x\}$ with $r(N') < r(N)$ that represents $C \setminus \{x\}$.

Lemma 3. Let $C = Cl(T)$ be a set of clusters on $\mathcal{X}$, where $T = \{T_1, T_2\}$ is a set of two binary trees on $\mathcal{X}$ with no non-trivial common subtrees, and $r(C) \geq 1$. Then for each $x \in \mathcal{X}$ it holds that $r(C) - 1 \leq r(C \setminus \{x\}) \leq r(C)$.

Proof. The second $\leq$ is immediate because removing a taxon from a cluster set cannot raise the reticulation number of the cluster set. The first $\leq$ holds because in \cite{2} it is shown how, given any network $N'$ on $\mathcal{X}' \setminus \{x\}$ that represents $C \setminus \{x\}$, we can extend $N'$ to obtain a network $N$ on $\mathcal{X}$ that represents $C$ such that $r(N) \leq r(N') + 1$.

Recall from \cite{2} the definition of an ST-set tree sequence of a cluster set $C$. Let $(S_1, S_2, ..., S_p)$ be an ST-set tree sequence of $C$ of minimum length, where $C = Cl(T) = Cl(T_1) \cup Cl(T_2)$. In \cite{2} it is proven that $p = r(C)$.

Lemma 4. Let $C = Cl(T)$ be a set of clusters on $\mathcal{X}$, where $T = \{T_1, T_2\}$ is a set of two binary trees on $\mathcal{X}$ with no non-trivial common subtrees, and $r(C) \geq 1$. Suppose there exist distinct taxa $a, b, c \in \mathcal{X}$ such that $\{a, b\}$ and $\{b, c\}$ are both clusters in $C$. Then there exists $x \in \{a, b, c\}$ such that $r(C \setminus \{x\}) = r(C) - 1$.

Proof. We know from \cite{2} that there exists an ST-set tree sequence $(S_1, ..., S_p)$ of $C$ where $p = r(C)$. It is clear that at least one of $\{a, b, c\}$ has to occur in one of the $S_i$ sets, because otherwise the two clusters $\{a, b\}$ and $\{b, c\}$ survive even after $S_i$ has been removed, contradicting the fact that it is a tree sequence. Now, let $1 \leq i \leq p$ be the smallest $i$ such that $S_i \cap \{a, b, c\} \neq \emptyset$. Note that, at the point just before the ST-set $S_i$ is removed, none of $\{a, b\}, \{b, c\}, \{a, c\}, \{a, b, c\}$ are ST-sets (because of the incompatible pair of clusters $\{a, b\}$ and $\{b, c\}$). So $|S_i \cap \{a, b, c\}| < 3$. Furthermore, $|S_i \cap \{a, b, c\}| \neq 2$ because at least one of the two clusters $\{a, b\}$ and $\{b, c\}$ will be incompatible with $S_i$. So $|S_i| = 1$ and $S_i \subseteq \{a, b, c\}$. Let $x$ be the single taxon in $S_i$. This means that $(S_1, ..., S_{i-1}, S_{i+1}, ..., S_p)$ is an ST-set tree sequence of $C \setminus \{x\}$ of length $p - 1$. We conclude that $r(C \setminus \{x\}) < r(C)$ and (by Lemma 3) we have that $r(C \setminus \{x\}) = r(C) - 1$.

Theorem 1. Let $C = Cl(T)$ be a set of clusters on $\mathcal{X}$, where $T = \{T_1, T_2\}$ is a set of two binary trees on $\mathcal{X}$ with no non-trivial common subtrees, and $r(C) \geq 1$. Then at least one of the following two conditions holds: (1) there exist distinct taxa $a, b, c \in \mathcal{X}$ such that $\{a, b\}$ and $\{b, c\}$ are both clusters in $C$; (2) there exists a taxon $x \in \mathcal{X}$ such that $r(C \setminus \{x\}) = r(C) - 1$ and $x$ is either a terminal of $C$ or is in some size-2 cluster with a terminal of $C$.

Proof. Towards a counter-example, assume that the claim does not hold for $C$. For each $x \in \mathcal{X}$ that is not a terminal, let $M(x)$ be an arbitrary terminal such that $x \rightarrow_C M(x)$, which must exist by Lemma 1. The mapping $M$ will remain unchanged for the rest of the proof.

Let $N$ be an arbitrary binary network that represents $C$ such that $r(N) = r(C)$. Due to the fact that $C$ is ST-collapsed, every SBR consists of exactly one taxon, so we can unambiguously identify each SBR by its corresponding taxon. Let $R(N) \subseteq \mathcal{X}$ be the set of SBRs of $N$. Clearly, if $R(N)$ contains a terminal we are done (by the same argument as used in the proof of Lemma 2).

For $x \in R(N)$, we define the detach and re-hang above a terminal (DRHT) operation as follows. We first delete $x$ and tidy up the resulting network in the usual fashion, which causes the parent reticulation of $x$ and its reticulation edges to disappear. This creates a network $N'$ on $\mathcal{X}' \setminus \{x\}$ that represents $C \setminus \{x\}$, where $r(N') = r(N) - 1$ (by Lemma 3). Let $\delta$ be the root of $N'$ and

\footnote{Note that Lemma 3 also prevents that, prior to the tidying-up phase, a multi-edge is created, because then both the parent reticulation of $x$ and the reticulation at the end of the multi-edge would disappear in the tidying-up phase, meaning that $r(N') \leq r(N) - 2$.}
Let \( p \) be the parent of \( M(x) \) in \( N' \). We construct a new network \( N'' \) from \( N' \) by deleting the edge \((p, M(x))\), introducing new nodes \( p', r, r' \), adding the edges \((p, p'), (p', M(x)), (p', r), (\delta, r), (r, r')\) and finally labeling \( r'\) with \( x \). This potentially raises the outdegree of the root above 2 (i.e. makes the network non-binary) but this could easily be addressed by replacing the root with a chain of nodes of indegree at most 1 and outdegree 2 (see e.g. [3]); the exposition is easier to follow if we permit a high-degree root. As observed in [2], let \( C \subseteq \mathcal{C} \) be a non-singleton cluster such that \( x \not\in C \). Clearly \( C \) is represented by \( N' \). The edge in \( N' \) that represents \( C \) will still represent \( C \) in \( N'' \) if we switch the reticulation edge \((p', r)\) off and the reticulation edge \((\delta, r)\) on. So suppose \( C \) is a non-singleton cluster that does contain \( x \). In this case \( M(x) \in C \setminus \{x\} \). So the edge in \( N' \) that represents \( C \setminus \{x\} \) can represent \( C \) in \( N'' \) by switching the reticulation edge \((p', r)\) on and the reticulation edge \((\delta, r)\) off. Hence \( N'' \) represents all clusters \( C \in \mathcal{C} \) and \( r(N'') = r(N) \). Note that, in general, \( R(N'') \neq R(N) \).

We will repeatedly apply the DRHT operation to transform \( N \) into a network with a "canonical" form. Specifically, choose an arbitrary \( x \in R(N) \) and let \( R^0 = \{x\} \). Let \( N^0 = N \) and let \( N^1 \) be the network obtained by applying the DRHT operation to \( x \) in \( N \). We apply the following procedure, starting with \( i = 0 \):

1. If \( R(N^{i+1}) \) contains a terminal then stop.
2. If \( R(N^{i+1}) \setminus R^i \neq \emptyset \) then stop.
3. Otherwise, let \( y \) be an arbitrary taxon in \( R(N^{i+1}) \setminus R^i \), let \( R^{i+1} = R^i \cup \{y\} \) and let \( N^{i+2} \) be obtained by applying the DRHT operation to \( y \) in \( N^{i+1} \). Increment \( i \) and go back to (1).

The procedure will definitely stop because with each new iteration \( |R^{i+1}| > |R^i| \). Let \( N^* \) be the final network obtained. Note that if the procedure stops at line (1) the proof is complete: \( N^* \) is a network that represents \( C \) with \( r(C) \) reticulations that has a terminal as a SBR. So we can assume that the procedure stops at line (2). Clearly, there are no terminals in \( R(N^*) \). Furthermore, for each \( x \in R(N^*) \) we know that at some iteration a DRHT operation was performed on \( x \), because otherwise the procedure could continue for at least one more iteration. In the iteration when this happens, the tail of one reticulation edge (of the parent reticulation of \( x \)) is attached to the root, and the other "just above" \( M(x) \) i.e. at \( p' \). In subsequent iterations \( M(x) \) will never undergo a DRHT operation, because it is a terminal. Also, \( x \) is not a terminal (and thus is not in the range of \( M \)) so the edge between \( x \) and its parent reticulation will never be subdivided by a DRHT operation. Furthermore, both reticulation edges will remain intact because, after the tidying-up phase, the DRHT operation only subdivides edges whose head is a taxon. In fact, the only relevant change that can happen is that the edge \((p', M(x))\) is subdivided by later DRHT operations; specifically, DRHT operations applied to some non-terminal \( y \neq x \) such that \( M(x) = M(y) \). Whether or not this happens, it follows that in \( N^* \) for every \( x \in R(N^*) \) one parent of the (parent reticulation of) \( x \) is the root, and the other parent is a node \( t(x) \) such that a directed tree-path (i.e. a path that contains no reticulations) exists from \( t(x) \) to \( M(x) \).

We will continue to focus on \( N^* \). We say that a directed path is a root-reticulation path if it starts at the root and terminates at a reticulation. The reticulation length of such a path is the number of reticulations in it (including the end node). Observe that the last node \( r \) on a root-reticulation path of maximum length must be (the parent reticulation of) an SBR. If this was not so then a previously unvisited reticulation \( r^* \neq r \) is reachable by a directed path from \( r \), thus contradicting the assumption that the root-reticulation path had maximum reticulation length.

Consider an arbitrary \( x' \in R(N^*) \) corresponding to the SBR at the end of a root-reticulation path of maximum reticulation length. Let \( x \) be the taxon in \( R(N^*) \) such that \( M(x) = M(x') \) and, amongst all such taxa, most recently underwent a DRHT operation; it might be that \( x = x' \). Note that, by construction, \( x \) is also at the end of a root-reticulation path of maximum reticulation length. Furthermore, one parent of (the parent reticulation of) \( x \) is the root, and the other is a node \( t(x) \) such that \((t(x), M(x))\) is an edge in \( N^* \). We are now ready for the core argument in the proof. We walk backwards from \( t(x) \) towards the root until we encounter a vertex \( u \) for which one of the following three mutually exclusive cases holds: (a) \( u \) is a reticulation; (b) \( u \) is a tree-node
Proof. Given that most taxon \( y \in X \setminus M(x) \) can be reached by a directed tree-path; (c) \( u \) is the root and (b) does not hold.

Before commencing with the case analysis we argue that \( N^* \) has a specific form. Let \( t \) be an intermediate node on the directed path from \( u \) to \( t(x) \). We know \( t \) is a tree-node from which no taxon (other than \( M(x) \)) can be reached by a directed tree-path. So all maximal directed tree-paths starting at \( t \) that do not terminate at \( M(x) \), must terminate at the parent of a reticulation \( r \). But then there exists a root-reticulation path of maximum reticulation length terminating at \( r \), so \( r \) is actually the parent of an SBR. Let \( x' \) be the taxon corresponding to this SBR. We know (by construction of \( N^* \)) that the non-root parent of \( r \) can reach \( M(x') \) by a directed tree-path. If \( M(x') \neq M(x) \) then (b) would actually have held for node \( t \), because merging the two directed tree-paths would create a directed tree-path from \( t \) to \( M(x') \), and the backwards walk would have terminated earlier. So \( M(x) = M(x') \) and hence \((t,r)\) is an edge in \( N^* \). From this we can conclude that, for each intermediate node \( t \), the child of \( t \) that does not lie on the path from \( u \) to \( t(x) \), is (the parent reticulation of) an SBR, and moreover all such SBRs map to \( M(x) \). We now commence the case analysis.

**Case (a).** In this case \( M(x) \) is the only taxon reachable by directed tree-paths from the child of reticulation \( u \). This is depicted in Figure 1. Consider the network \( N^{**} \) obtained from \( N^* \) by deleting \( M(x) \) and suppressing its parent; in particular, consider how this changes Figure 1. Clearly, \( N^{**} \) represents \( C \setminus \{M(x)\} \). Now, there is some ST-set tree sequence of \( C \setminus \{M(x)\} \) that begins \( \{x, \{x_1\}, \ldots, \{x_n\}\} \), because singletons are always ST-sets. Each time one of these ST-sets is removed from \( N^{**} \) the reticulation number of \( N^{**} \) drops by exactly one, except at the point when \( \{x''\} \) is removed, because at this point the reticulation \( u \) will also disappear, causing the reticulation number of the network to drop by two. Hence we can conclude that \( C \setminus \{M(x)\} \) has an ST-set tree sequence of length \( r(N^*) - 1 = r(C) - 1 \), and we are done.

**Case (b).** Let \( y \neq M(x) \) be the taxon that can be reached by a directed tree-path from \( u \). This is depicted in Figure 2. \( M(x) \) is a terminal, so there must exist some non-singleton cluster \( C \in \mathcal{C} \) such that \( M(x) \in C \), but \( y \) is not in \( C \). Critically, the only edges that can represent such a cluster lie on the path from \( u \) to \( t(x) \). Hence there exists \( R' \subseteq R(N^*) \) such that \( C = R' \cup M(x) \) and for all \( x' \in R' \), \( M(x') = M(x) \). So for each \( x' \in R' \) we know that \( x' \rightarrow_{C} M(x) \). Hence in both \( T_1 \) and \( T_2 \) the parent of \( M(x) \) must be reachable by a directed path from the parent of \( x' \) (possibly of length 0). Suppose there exist \( y', z' \in X \) such that \( y' \in W^{T_1}(M(x)), z' \in W^{T_2}(M(x)) \) and neither \( y' \) nor \( z' \) is in \( R' \). But then every non-singleton cluster in \( C \) that contains \( M(x) \), contains either \( y' \) or \( z' \). Hence \( C \not\subseteq C \), which is obviously not possible. So there must be some element \( x'' \in R' \) that appears in (wlog) \( W^{T_1}(M(x)) \). But there must also be a directed path from the parent of \( x'' \) to the parent of \( M(x) \) in \( T_1 \). So \( x'' \) must be a sibling of \( M(x) \), i.e. \( \{x'', M(x)\} \in C \). Furthermore, \( x'' \) is an SBR, and \( M(x) \) is a terminal, so we are done.

**Case (c).** In this case the network must look like Figure 3 because the maximum reticulation length of a root-reticulation path is 1. \( M(x) \) is in at least one non-singleton cluster \( C \) (otherwise it would not be a terminal) so there again exists \( R' \subseteq R(N^*) \) such that \( C = R' \cup M(x) \) and for all \( x' \in R' \), \( M(x') = M(x) \). (In this case \( R(N^*) = X \setminus \{M(x)\} \)). The rest of the analysis is the same as case (b).

**Lemma 5.** Let \( C \) be an ST-collapsed set of clusters on \( X \) such that \( r(C) \geq 1 \). Then \( C \) contains at most \( 3 \cdot r(C) \) terminals.

**Proof.** Given that \( C \) is ST-collapsed, we know that there exists a binary network \( N \) with \( r(N) = r(C) \) that represents \( C \) such that \( N \) can be obtained by performing the leaf-hanging operation to some \( r(C) \)-reticulation generator \([1]\). The 1-reticulation and 2-reticulation generators are shown in Figure 4. Recall that the edges of a generator are called edge sides and that the nodes of a generator with indegree-2 and outdegree-0 are called node sides. For a generator \( G \) we let \( I(G) \) be
Fig. 1. This is case (a) in the proof of Theorem 1. Here \( u \) is a reticulation and the only taxon reachable by a directed tree-path from the child of \( u \) is \( M(x) \). Each intermediate node on the path from \( u \) to \( M(x) \) is the tail of a reticulation edge that feeds into (the parent reticulation of) an SBR; the other reticulation edge is attached to the root. All these SBRs \( x, x', ..., x'' \) are such that \( M(x) = M(x') = ... = M(x'') \).

Fig. 2. This is case (b) in the proof of Theorem 1. Here \( u \) is a tree-node and there is a taxon \( y \neq M(x) \) reachable by a directed tree-path from \( u \). Each intermediate node on the path from \( u \) to \( M(x) \) is the tail of a reticulation edge that feeds into (the parent reticulation of) an SBR; the other reticulation edge is attached to the root. All these SBRs \( x, x', ..., x'' \) are such that \( M(x) = M(x') = ... = M(x'') \).
Fig. 3. This is case (c) in the proof of Theorem 1. Here $u$ is the root and $X = \{x, x', \ldots, x''\} \cup \{M(x)\}$. Each intermediate node on the path from $u$ to $M(x)$ is the tail of a reticulation edge that feeds into (the parent reticulation of) an SBR; the other reticulation edge is attached to the root. All these SBRs $x, x', \ldots, x''$ are such that $M(x) = M(x') = \ldots = M(x'')$.

any maximum size subset of edge sides such that, for every two sides $s \neq s'$ in $I(G)$, there is no directed path from the head of $s$ to the tail of $s'$ such that all nodes on the path (including the head of $s$ and the tail of $s'$) are tree-nodes. We let $R(G)$ be the set of node sides of $G$, and we define $t(G)$ as $|R(G)| + |I(G)|$. We define $t(r)$ (where $r \geq 1$) as the maximum value of $t(G)$ ranging over all $r$-reticulation generators $G$. Observe that, if $r(\mathcal{C}) = r$, then $t(r)$ is an upper bound on the number of terminals in $\mathcal{C}$. This follows because there can be at most one terminal per edge side and, more generally, it is not possible to place two terminals $x \neq y$ on the sides of the generator such that a directed tree-path exists from the parent of $x$ to the parent of $y$, because then $x \rightarrow_{\mathcal{C}} y$. To prove the lemma we will show that $t(r) \leq 3r$ for $r \geq 1$.

We will prove this by induction. The base case $r = 1$ is straightforward. There can be at most three terminals placed on the 1-reticulation generator; one on the node side and one on each of the two edges whose head is the node side, see Figure [4]. (The cluster set $\mathcal{C} = \{\{a, b\}, \{b, c\}, \{d, c\}, \{e, d\}\}$, for which $r(\mathcal{C}) = 1$, shows that three terminals is actually possible).

Observe that, by acyclicity, every generator has at least one node side. Furthermore, if we (1) delete a node side $s$ from an $r$-reticulation generator, (2) delete all leaves that are created (nodes with indegree-1 and outdegree-0) and (3) suppress all nodes with indegree and outdegree both equal to 1, we obtain an $(r-1)$-reticulation generator. For example, observe how applying steps (1)-(3) to any 2-reticulation generator creates the unique 1-reticulation generator.

Now, for the sake of contradiction assume that $r > 1$ is the smallest value such that $t(r) > 3r$. Let $G$ be an $r$-reticulation generator such that $t(G) \geq 3r + 1$. Let $I(G)$ be a subset of the edge sides, as defined above, such that $t(G) = |R(G)| + |I(G)|$. Locate an arbitrary node side $s$ of $G$. We will show that deleting $s$ and applying steps (1)-(3) as described above will create an $(r-1)$-generator $G'$ such that $t(G') \geq t(G) - 3$, yielding a contradiction on the assumed minimality of $r$. There are several cases, conditional on the positions of the tails of the two edges that enter $s$.

In case (i) the two tails are distinct and both have indegree-2 and outdegree-1. In this case, by the maximality of $I(G)$, both the edges entering $s$ will be in $I(G)$. Hence, $|I(G')| = |I(G)| - 2$ and $|R(G')| = |R(G)| + 1$, so $t(G') = t(G) - 1$.

In case (ii) the two tails are distinct and both have indegree-1 and outdegree-2. Clearly $|R(G')| = |R(G)| - 1$. Let $u$ be the tail of the first edge that enters $s$. Let $p(u)$ be the parent of $u$ and $c(u)$ the child of $u$ not equal to $s$. The critical observation is that at most one of $(u, c(u))$ and $(p(u), u)$ is
in $I(G)$. So deleting $s$ will delete the edge $(u, s)$ from $I(G)$, if it is there, and if one of $(u, c(u))$ and $(p(u), u)$ is in $I(G)$ then this can be deleted and replaced by the new edge $(p(u), c(u))$. The same analysis holds for the second edge $(v, s)$ entering $s$. Hence $|I(G')| \geq |I(G)| - 2$, and this completes this case. Note that the analysis still holds if (wlog) $p(v) = u$, because then at most one of the three edges $(p(u), u), (u, v), (v, c(v))$ will be in $I(G)$, and if this occurs this edge can be replaced by the new edge $(p(u), c(v))$.

In case (iii) both tails are distinct, one tail has indegree-2 and outdegree-1 and the other tail has indegree-1 and outdegree-2. Then, by combining the insights from the first two cases, $|R(G')| = |R(G)|$ and $|I(G')| \geq |I(G)| - 2$.

Finally, in case (iv) the two tails are the same vertex $u$ i.e. $s$ is the head of a multi-edge. Note that at most two of the three edges $(p(u), u), (u, s), (u, s)$ can be in $I(G)$. Now, suppose $p(u)$ has indegree-2 and outdegree-1. Then $|R(G')| = |R(G)|$ and $|I(G')| \geq |I(G)| - 2$. In the case that $p(u)$ has indegree-1 and outdegree-2 we have that $|R(G')| = |R(G)| - 1$, and let $p'$ be the parent of $p(u)$ and $c'$ be the child of $p(u)$ not equal to $u$. Again, at most one of the two edges $(p', p(u))$ and $(p(u), c')$ will be in $I(G)$, and if necessary this can be replaced by the new edge $(p', c')$. So $|I(G')| \geq |I(G)| - 2$.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure.png}
\caption{The single 1-reticulation generator and the seven 2-reticulation generators.}
\end{figure}

Lemma 6. Let $C = Cl(T)$ be a set of clusters on $\mathcal{X}$, where $T = \{T_1, T_2\}$ is a set of two binary trees on $\mathcal{X}$ with no non-trivial common subtrees, and $r(C) \geq 1$. Then there exists $\mathcal{X}' \subseteq \mathcal{X}$ such that (1) $|\mathcal{X}'| \leq 6 \cdot r(C)$ and (2) there exists $x \in \mathcal{X}'$ such that $r(C \setminus \{x\}) = r(C) - 1$. Furthermore such a set $\mathcal{X}'$ can be computed in polynomial time.
Proof. If situation (1) from the statement of Theorem 1 holds then we can simply take $X' = \{a, b, c\}$, so $|X'| = 3 \leq 6 \cdot r(C)$. Otherwise we are in situation (2) and we take $X'$ to be the union of all terminals of $C$ plus all taxa that appear in some size-2 cluster of $C$ with some terminal. From Lemma 5 we know that there are at most $3 \cdot r(C)$ terminals in $C$. Observe that each such terminal can be in at most one size-2 cluster, because otherwise there would exist two incompatible size-2 clusters i.e. situation (1) of Theorem 1 would hold. Hence there can be at most $3 \cdot r(C)$ non-terminals that appear in size-2 clusters with terminals, from which $|X'| \leq 6 \cdot r(C)$ follows.

Given the characterisation described in Observation 2 and the fact that $|C| \leq 4(n - 1)$, it is easy to see that the set $X'$ can be computed in (low-order) polynomial time.

Theorem 2. Let $C = Cl(T)$ be a set of clusters on $X$, where $T = \{T_1, T_2\}$ is a set of two binary trees on $X$. Then $r(C) = h(T)$ can be computed in time $(6r)^r \cdot \text{poly}(n)$ time, where $r = r(C)$ and $n = |X|$.

Proof. The algorithm is simple. We repeat the following steps until a compatible cluster set (i.e. a set of clusters that can be represented by a tree) is created: (1) collapse any common subtrees into single taxa (adjusting $C$ as necessary), this can be done in (low-order) polynomial time, (2) construct the set $X'$ described in Lemma 6 and then (3) “guess” an element $x \in X'$ such that $r(C \setminus \{x\}) = r(C) - 1$.

At each iteration the guessing can be simulated simply by trying all (at most) $6r$ elements in $X'$. (Note that the $X'$ sets that arise will never have more than $6r$ elements because removing taxa from a cluster set cannot raise the reticulation number of the cluster set). If we traverse this search tree in breadth-first fashion and stop as soon as we have created a compatible cluster set then the depth of the search tree will equal $r = r(C)$, requiring at most $\Theta((6r)^r)$ guesses in total.

3 Conclusion

We have presented a new fixed parameter tractable algorithm for computing the hybridization number of two binary phylogenetic trees. The algorithm is unusual in the sense that it attacks the problem indirectly: it works within the softwired clusters model (which does not require the full topology of the input trees to be preserved) and links the optima together using the unification results in [3,2]. We hope that this will stimulate new insights into the underlying combinatorial structure of the hybridization number problem.

References

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