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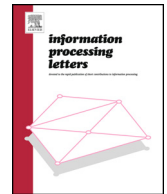
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Cyclic generators and an improved linear kernel for the rooted subtree prune and regraft distance



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ABSTRACT

The rooted subtree prune and regraft (rSPR) distance between two rooted binary phylogenetic trees is a well-studied measure of topological dissimilarity that is NP-hard to compute. Here we describe an improved linear kernel for the problem. In particular, we show that if the classical subtree and chain reduction rules are augmented with a modified type of chain reduction rule, the resulting trees have at most $9k - 3$ leaves, where k is the rSPR distance; and that this bound is tight. In comparison, the previous best-known linear kernel is of size at most $28k$. To achieve this improvement we introduce cyclic generators, which can be viewed as cyclic analogues of the generators used in the phylogenetic networks literature. As a corollary to our main result we also give an improved weighted linear kernel for the minimum hybridization problem on two rooted binary phylogenetic trees.

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1. Introduction

The central challenge of phylogenetics is to infer the evolutionary history of a set of contemporary species X . Often this history is modeled by a *rooted phylogenetic tree*; essentially, a rooted tree in which the leaves are bijectively labeled by X and evolution is explicitly directed away from the root [16]. Due to confounding biological or methodological factors the inferred trees sometimes differ in topology, and then it is useful to formally quantify these differences [10]. One popular such difference measure is the *rooted subtree prune and regraft* (rSPR) distance. Informally this measures the number of times that a subtree

must be pruned, and re-attached, to transform one tree into another. Despite the NP-hardness of computing this distance [3], very fast fixed-parameter tractable branching algorithms have been developed which allow the problem to be well solved in practice, as long as the rSPR distance does not become too large [20,21]. A related concept is *kernelization*: polynomial-time pre-processing rules which reduce the size of the input trees to purely a function of their rSPR distance [8]. Compared to branching algorithms there has been relatively little work on kernelization of rSPR. Indeed, currently the best-known result is that after exhaustive application of the *subtree* and *chain* reduction rules the input trees have at most $28k$ leaves, where k is the rSPR distance [3].

In this paper, we show that when a third, modified chain reduction rule is added to the portfolio, the bound improves to $9k - 3$, and that this is in fact tight. To prove this we first show that computation of rSPR distance is essentially equivalent to the problem of parsimoniously embedding the two input trees into a potentially cyclic phylogenetic network (i.e. graph); it is a cyclic variant of the

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much-studied *minimum hybridization* problem (see e.g. [17] and links therein). This allows us to introduce *cyclic generators* which summarize the backbone of such networks, and allow us to carefully bound the size of reduced instances. Our approach is inspired by a similar strategy which has proven to be very powerful in the design of reduction rules for *unrooted* phylogenetic trees [12]. As a corollary to our main rSPR result, we also show that the three aforementioned reduction rules yield a weighted linear kernel of $7k - 2$ for the minimum hybridization problem, where k is the hybridization number of the two trees. This improves upon the weighted $9k - 2$ kernel given in [13].

2. Preliminaries

Throughout this paper, X denotes a non-empty finite set.

Phylogenetic trees. A *rooted phylogenetic X -tree* T is a rooted tree with no degree-2 vertex, except for the root which has degree at least 2, and whose leaf set is X . All edges of T are directed away from the root, i.e. if (u, v) is an edge of T , then u lies on the directed path from the root of T to v . Furthermore, T is *binary* if its root has degree 2 and all other interior vertices have degree 3. The leaf set X is the *label set* of T and denoted by $L(T)$. For two vertices u and v in T , we say that u is an *ancestor* of v if there is a directed path from the root of T to v that contains u . We next define three types of subtrees of T relative to a subset $X' \subseteq X$. First, we write $T[X']$ to denote the minimal rooted subtree of T that connects all elements in X' . Second, the *restriction* of T to X' , denoted by $T|X'$, is the rooted phylogenetic X' -tree obtained from $T[X']$ by suppressing all vertices with in-degree 1 and out-degree 1. Lastly, a rooted subtree of T is *pendant* if it can be detached from T by deleting a single edge. Since all rooted phylogenetic trees throughout this paper are binary, we refer to a rooted binary phylogenetic tree simply as a *rooted phylogenetic tree*. For two rooted phylogenetic X -trees T and T' , we say that T and T' are *isomorphic* if there is a bijection ϕ from the vertex set V of T to the vertex set of T' such that $\phi(x) = x$ for each $x \in X$, and (u, v) is an edge of T if and only if $(\phi(u), \phi(v))$ is an edge of T' for all $u, v \in V$. If T and T' are isomorphic, we write $T = T'$.

rSPR and agreement forests. Let T be a rooted phylogenetic X -tree. For the purposes of the upcoming definitions and indeed much of the paper, we view the root of T as a vertex ρ adjoined to the original root by a pendant edge. Furthermore, we regard ρ as part of the label set of T , that is $L(T) = X \cup \{\rho\}$. Fig. 1 illustrates an example of two rooted phylogenetic X -trees with $X = \{x_1, x_2, \dots, x_6\}$ with their roots labeled with ρ . Let $e = (u, v)$ be an edge of T not incident with ρ . Let T' be the rooted phylogenetic X -tree obtained from T by deleting e and re-attaching the resulting rooted subtree containing v via a new edge f as follows. Subdivide an edge of the component that contains ρ with a new vertex u' , join u' and v with f , and suppress u . We say that T' has been obtained from T by a *rooted subtree prune and regraft* (rSPR) operation. The rSPR distance between any two rooted phylogenetic X -trees T and T' , denoted by $d_{\text{rSPR}}(T, T')$, is the minimum number of rSPR operations that transform T into T' . It is well known that

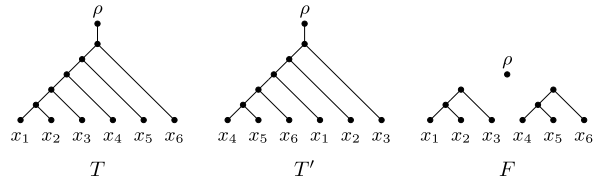


Fig. 1. Two rooted phylogenetic trees T and T' with their roots labeled ρ , and an agreement forest F for T and T' . All edges are directed downwards.

one can always transform T into T' via a sequence of rSPR operations. However, computing $d_{\text{rSPR}}(T, T')$ is an NP-hard problem [3,9].

Now, let T and T' be two rooted phylogenetic X -trees. An *agreement forest* $F = \{L_\rho, L_1, \dots, L_k\}$ for T and T' is a partition of $X \cup \{\rho\}$ such that $\rho \in L_\rho$ and the following two properties are satisfied:

- (P1) For all $i \in \{\rho, 1, \dots, k\}$, we have $T|L_i = T'|L_i$.
- (P2) The trees in $\{T|L_i : i \in \{\rho, 1, \dots, k\}\}$ and $\{T'|L_i : i \in \{\rho, 1, \dots, k\}\}$ are vertex-disjoint subtrees of T and T' , respectively.

An agreement forest for T and T' is a *maximum agreement forest* if, amongst all agreement forests for T and T' , it has the smallest number of elements. To illustrate, Fig. 1 shows an agreement forest F for the two rooted phylogenetic trees T and T' of the same figure. Indeed, F is a maximum agreement forest for T and T' . The following theorem characterizes the rSPR distance between two rooted phylogenetic trees (with their roots labeled ρ) in terms of agreement forests.

Theorem 2.1. [3] *Let T and T' be two rooted phylogenetic X -trees, and let F be a maximum agreement forest for T and T' . Then $d_{\text{rSPR}}(T, T') = |F| - 1$.*

3. Leaf-labeled graphs characterize the rSPR distance

In this section, we establish an alternative characterization for the rSPR distance between two rooted phylogenetic trees. A *rooted leaf-labeled graph* G on X is a rooted directed graph with no parallel edges or loops that satisfies the following four properties:

- (i) the unique root has in-degree 0 and out-degree 1, and is labeled ρ ,
- (ii) a vertex of out-degree 0 has in-degree 1, and the set of vertices with out-degree 0 is X ,
- (iii) all other vertices either have in-degree 1 and out-degree 2, or in-degree 2 and out-degree 1, and
- (iv) each vertex can be reached from ρ via a directed path.

A vertex of G with in-degree 1 and out-degree 2 is a *tree vertex*, while a vertex of in-degree 2 and out-degree 1 is a *reticulation*. For two vertices u and v in G , we say that u is a *parent* of v if (u, v) is an edge. In contrast to a rooted phylogenetic network [10,16], observe that G may contain a directed cycle. Nevertheless, as in the case of rooted (binary) phylogenetic networks, the number of reticulations

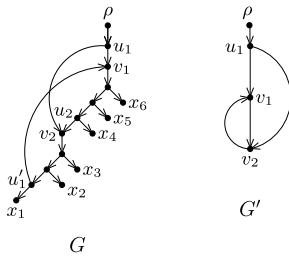


Fig. 2. Left: A rooted leaf-labeled graph G that displays the two rooted phylogenetic trees T and T' that are shown in Fig. 1. The reticulations of G are v_1 and v_2 . To see that G displays T' , note that the graph obtained from G by deleting the two edges (u_1, v_1) and (u_2, v_2) is a subdivision of T' . Right: The cyclic 2-generator G' that underlies G . To obtain G from G' , the elements in $\{x_1, x_2, x_3\}$ are attached to the side (v_2, v_1) and the elements in $\{x_4, x_5, x_6\}$ are attached to the side (v_1, v_2) .

in $G = (V, E)$, denoted $r(G)$, is equal to $|E| - (|V| - 1)$. This is because G , due to property (iv), has a directed spanning tree, rooted at ρ , with $|V| - 1$ edges. The spanning tree does not yet have any vertices with in-degree 2. Each of the $|E| - (|V| - 1)$ edges from E that are not on the spanning tree, creates exactly one in-degree 2 vertex when added to it. Hence, there are exactly $|E| - (|V| - 1)$ reticulations in total.

As for rooted phylogenetic trees, a rooted subtree of G is *pendant* if it can be detached from G by deleting a single edge. Let T and T' be two rooted phylogenetic X -trees. We say that T is *displayed* by G if there exists a subgraph of G that is a subdivision of T . Moreover we set

$$r^\circ(T, T') = \min_G \{r(G)\}.$$

That is, $r^\circ(T, T')$ equates to the minimum number of reticulations over all rooted leaf-labeled graphs that display T and T' . Fig. 2 shows a rooted leaf-labeled graph G that displays the two rooted phylogenetic trees T and T' that are depicted in Fig. 1. Note that $r(G) = 2 = d_{\text{rSPR}}(T, T')$. The next theorem shows that this relationship is not a coincidence. We note that the idea of viewing a sequence of rSPR operations as a rooted leaf-labeled graph was briefly mentioned in [15] for the purpose of highlighting that such a graph may contain a directed cycle.

Theorem 3.1. *Let T and T' be two rooted phylogenetic X -trees. Then $d_{\text{rSPR}}(T, T') = r^\circ(T, T')$.*

Proof. Throughout this proof, we continue with our convention that trees and graphs have an in-degree 0, out-degree 1 root labeled ρ .

We first show that $r^\circ(T, T') \geq d_{\text{rSPR}}(T, T')$. This part of the proof is similar to the second part of the proof of [18]. Let G be a rooted leaf-labeled graph on X that displays T and T' such that $r(G) = r^\circ(T, T')$. Let $V(G)$ and $E(G)$ be the vertex and edge set of G , respectively. Let E_T be the edge set of a subdivision of T in G . Similarly, let $E_{T'}$ be the edge set of a (directed) spanning tree of G that is obtained from a subdivision of T' in G by adding a possibly empty set of edges. Note that $|E_{T'}| = |V(G)| - 1$, and that both E_T and $E_{T'}$ contain the edge of G that is incident with ρ .

Lastly, let A be the subset of E_T that contains precisely each edge that is not in $E_{T'}$. We next obtain two graphs from G . First, obtain G' from G by deleting each edge in A . Observe that the edge set of G' contains each edge in $E_{T'}$ and, hence $|E(G')| - |V(G)| \geq |V(G)| - 1$. It therefore follows that

$$|A| \leq |E(G)| - |V(G)| + 1 = r(G). \tag{1}$$

Second, obtain F from G by deleting each edge that is not in E_T , deleting each edge in A , deleting each of the resulting connected components that does not contain at least one vertex labeled with an element in $X \cup \{\rho\}$, and applying any of the following operations until no further operation is possible.

1. Delete each vertex with in-degree 0 and out-degree 1 that is not ρ .
2. Delete each unlabeled vertex with out-degree 0.
3. Suppress each vertex with in-degree 1 and out-degree 1.

By construction, F has at most $|A| + 1$ elements. Furthermore, the partition of $X \cup \{\rho\}$ in which each block corresponds to the label set of an element in F is an agreement forest for T and T' . Hence,

$$d_{\text{rSPR}}(T, T') \leq |F| - 1 \leq |A| \leq r(G) = r^\circ(T, T'),$$

where the first inequality follows from Theorem 2.1 and the third inequality follows from Equation (1).

We complete the proof by showing that $r^\circ(T, T') \leq d_{\text{rSPR}}(T, T')$. This part of the proof is by induction on $d_{\text{rSPR}}(T, T')$. If $d_{\text{rSPR}}(T, T') = 0$, then $G = T = T'$ is a rooted leaf-labeled graph with $r(G) = 0$ that displays T and T' . Assume that $d_{\text{rSPR}}(T, T') = k$ and that the theorem holds for all pairs of rooted phylogenetic trees whose rSPR distance is at most $k - 1$. Then there exists a rooted phylogenetic X -tree T'' such that $d_{\text{rSPR}}(T, T'') = k - 1$ and $d_{\text{rSPR}}(T'', T') = 1$. (If $k = 1$, then $T = T''$.) By the induction assumption, there exists a rooted leaf-labeled graph G' on X with $r(G') \leq k - 1$ that displays T and T'' .

We next construct a rooted leaf-labeled graph G from G' . Let $E_{T''}$ be the edge set of a subdivision of T'' in G' . Consider the rSPR operation that transforms T'' into T' . Let f be the edge that is deleted in T'' and let f' be the edge that is subdivided after the deletion of f . Then f (resp. f') corresponds to a directed path P (resp. P') in $E_{T''}$. Let e (resp. e') be an edge of P (resp. P'). Now obtain G from G' by subdividing e with a new vertex v_1 , subdividing e' with a new vertex v_2 , and adding the edge (v_2, v_1) . Clearly as G' is a rooted leaf-labeled graph on X , G is also such a graph with $r(G) = r(G') + 1$. Moreover, as G' displays T and T'' , it follows from the construction that G displays T and T' . Hence

$$\begin{aligned} d_{\text{rSPR}}(T, T') &= d_{\text{rSPR}}(T, T'') + d_{\text{rSPR}}(T'', T') \\ &\geq r(G') + 1 = r(G) \geq r^\circ(T, T'). \quad \square \end{aligned}$$

4. Cyclic generators

Let $k \geq 1$ be a positive integer. A *cyclic k -generator* (or short *cyclic generator* if k is clear from the context) is a connected directed graph that may contain parallel edges but no loops, and that satisfies the following four properties:

- (i) the unique root is labeled ρ and has in-degree 0 and out-degree 1,
- (ii) there are exactly k vertices with in-degree 2 and out-degree at most 1,
- (iii) all other vertices have in-degree 1 and out-degree 2, and
- (iv) each vertex can be reached from ρ via a directed path.

The *sides* of a cyclic k -generator are its edges, called the *edge sides*, and its vertices of in-degree 2 and out-degree 0, called the *vertex sides*.

Now, let G be a rooted leaf-labeled graph with $r(G) = k$ that has no pendant subtree with at least two leaves. Then, we can obtain a cyclic k -generator G' from G by deleting all leaves and suppressing each resulting vertex with in-degree 1 and out-degree 1. We say that G' is the cyclic k -generator that *underlies* G . Reversely, the edge and vertex sides of a cyclic generator are the places where leaves can be attached to obtain a rooted leaf-labeled graph. More precisely, let $Y = \{y_1, y_2, \dots, y_m\}$ be a set of leaves, and let G' be a cyclic k -generator. Then, *attaching* Y to an edge side (u, v) of G' is the operation of subdividing (u, v) with m vertices w_1, w_2, \dots, w_m and, for each $i \in \{1, 2, \dots, m\}$, adding an edge (w_i, y_i) . Moreover, *attaching* Y to a vertex side v of G' is the operation of adding an edge (v, r) , where r is the root of a rooted phylogenetic Y -tree. If at least one new leaf is attached to each pair of parallel edges and to each vertex side in G' , then the resulting graph is a rooted leaf-labeled graph G with $r(G) = k$. We summarize the construction in the next observation.

Observation 4.1. *Let G be a rooted leaf-labeled graph that has no pendant subtree with at least two leaves, and let G' be a cyclic $r(G)$ -generator. Then G' underlies G if and only if G can be obtained from G' by attaching a (possibly empty) set of leaves to each edge and vertex side of G .*

As an example, Fig. 2 shows the cyclic 2-generator G' that underlies the rooted leaf-labeled graph G that is depicted in the same figure.

The proof of the next lemma was first established for generators without any directed cycle in [13]. However, the same proof applies without any changes to cyclic k -generators.

Lemma 4.2. *Let $k \geq 1$, and let G' be a cyclic k -generator. Then G' has $4k_0 + 3k_1 - 1$ edge sides, where k_0 is the number of vertex sides in G' and k_1 is the number of vertices in G' with in-degree 2 and out-degree 1.*

5. Reductions

This section describes three reductions that can be applied to two rooted phylogenetic trees to shrink them to two smaller trees before computing their rSPR distance. The first two reductions were established in [3], where the authors have shown that each reduction preserves the rSPR distance. The third reduction, which was established in [20] in the context of a depth-bounded search tree algorithm for computing the rSPR distance reduces the rSPR distance by 1.

Let T be a rooted phylogenetic X -tree, and let $C = (x_1, x_2, \dots, x_n)$ be a sequence of elements in X with $n \geq 2$. We say that C is an *n -chain* (or short *chain*) of T if the parent of x_1 coincides with the parent of x_2 or the parent of x_2 is the parent of the parent of x_1 , and, for each $i \in \{3, 4, \dots, n\}$, the parent of x_i is the parent of the parent of x_{i-1} . By definition, no chain of T contains ρ . If C is a chain of T and the parent of x_1 coincides with the parent of x_2 , then we say that C is *pendant* in T , in which case $C = (x_1, x_2, x_3, \dots, x_n) = (x_2, x_1, x_3, \dots, x_n)$. If a chain is a chain of both T and T' , we say that it is a *common chain*. Referring back to Fig. 1, we note that T and T' as shown in this figure have two common 3-chains (x_1, x_2, x_3) and (x_4, x_5, x_6) and each is pendant in one of T and T' .

Let T and T' be two rooted phylogenetic X -trees. We next describe three reductions to obtain two rooted phylogenetic trees S and S' from T and T' , respectively, with fewer leaves.

Subtree reduction. For $m \geq 2$, let $\{x_1, x_2, \dots, x_m\}$ be the leaf set of a maximal pendant subtree that is common to T and T' . Then set $S = T|X \setminus \{x_2, x_3, \dots, x_m\}$ and $S' = T'|X \setminus \{x_2, x_3, \dots, x_m\}$.

Chain reduction. For $n \geq 4$, let $C = (x_1, x_2, \dots, x_n)$ be a maximal n -chain that is common to T and T' . Then set $S = T|X \setminus \{x_4, x_5, \dots, x_n\}$ and $S' = T'|X \setminus \{x_4, x_5, \dots, x_n\}$.

3-2-chain reduction. Let (x_1, x_2, x_3) be a pendant 3-chain of T . If (x_i, x_3) is a pendant 2-chain in T' with $x_i \in \{x_1, x_2\}$, then set $S = T|X \setminus \{x_j\}$ and $S' = T'|X \setminus \{x_j\}$ with $\{x_i, x_j\} = \{x_1, x_2\}$.

Note that after an application of the 3-2-chain reduction, (x_i, x_3) is a pendant 2-chain that is common to S and S' . It can therefore be further reduced by a subtree reduction.

The next lemma shows that an application of the 3-2-chain reduction reduces the rSPR distance by 1. A slightly more general result was established in [20], where the authors applied the reduction to two forests instead of two rooted phylogenetic trees. To keep the exposition self contained, we include a full proof that is adapted to the setting of our paper.

Lemma 5.1. *Let T and T' be two rooted phylogenetic X -trees, and let S and S' be two trees obtained from T and T' , respectively, by a single application of the 3-2-chain reduction. Then $d_{\text{rSPR}}(S, S') = d_{\text{rSPR}}(T, T') - 1$.*

Proof. Without loss of generality, we establish the lemma using the same notation as in the definition of a 3-2-chain reduction. Let F_S be a maximum agreement forest for S

and S' , and let F_T be a maximum agreement forest for T and T' . Then $F_S \cup \{\{x_j\}\}$ is an agreement forest for T and T' , which implies that $|F_S| + 1 \geq |F_T|$. Hence

$$d_{\text{rSPR}}(S, S') = |F_S| - 1 \geq |F_T| - 2 = d_{\text{rSPR}}(T, T') - 1.$$

Now consider F_T . If $\{x_j\} \in F_T$ then $F \setminus \{\{x_j\}\}$ is an agreement forest for S and S' , so $d_{\text{rSPR}}(S, S') \leq d_{\text{rSPR}}(T, T') - 1$ and we are done. Assume therefore that $\{x_j\} \notin F_T$. Let B be the element in F_T , with $|B| \geq 2$, that properly contains x_j . Then (P2) in the definition of an agreement forest implies that x_i and x_3 cannot both be contained in B . We next consider three cases.

First, assume that $x_3 \in B$ and $x_i \notin B$. Then $\{x_i\} \in F_T$. Let $B' = (B \setminus \{x_j\}) \cup \{x_i\}$. Since $T|B = T'|B$, it follows that

$$(F_T \setminus \{B, \{x_i\}\}) \cup \{\{x_j\}, B'\}$$

is a maximum agreement forest for T and T' . Second, assume that $x_i \in B$ and $x_3 \notin B$. Then $\{x_3\} \in F_T$ and an argument that is similar to that used in the first case implies that there exists a maximum agreement forest for T and T' in which $\{x_j\}$ is an element. Third, assume that $x_i, x_3 \notin B$. Then, as F_T satisfies (P2), $\{x_i\}$ and $\{x_3\}$ are both elements in F_T . Hence

$$(F_T \setminus \{B, \{x_i\}, \{x_3\}\}) \cup \{\{x_i, x_3\}, \{x_j\}, B \setminus \{x_j\}\}$$

is a maximum agreement forest for T and T' .

Taken together, the three cases described in the last paragraph show that there exists another maximum agreement forest for T and T' in which $\{x_j\}$ is an element. We may therefore assume that F_T is indeed such a forest. This implies that $F_T \setminus \{\{x_j\}\}$ is an agreement forest for S and S' with $|F_S| \leq |F_T| - 1$ and, so,

$$d_{\text{rSPR}}(T, T') - 1 = |F_T| - 2 \geq |F_S| - 1 = d_{\text{rSPR}}(S, S').$$

Combining both cases establishes the lemma. \square

6. A new kernel for rSPR distance

The current smallest kernel size for computing the rSPR distance as stated in the next lemma was established in 2005 [3].

Lemma 6.1. *Let S and S' be two rooted phylogenetic X -trees. Suppose that S and S' cannot be reduced any further by applying the subtree or chain reduction. Then $|X| \leq 28d_{\text{rSPR}}(S, S')$.*

We next show that the size of the rSPR kernel can be substantially improved by additionally applying the 3-2-chain reduction.

Theorem 6.2. *Let S and S' be two rooted phylogenetic X -trees such that $d_{\text{rSPR}}(S, S') \geq 1$. Suppose that S and S' cannot be reduced any further by applying the subtree, chain, or 3-2-chain reduction. Then $|X| \leq 9d_{\text{rSPR}}(S, S') - 3$.*

Proof. Let G be a rooted leaf-labeled graph on X that displays S and S' such that $r(G) = r^\circ(S, S') = d_{\text{rSPR}}(S, S') =$

$k \geq 1$, where the second equality follows from Theorem 3.1. Let G' be the cyclic k -generator that underlies G . Now G can be obtained from G' by attaching leaves in X to the edge and vertex sides of G' . In what follows we bound the number of leaves that can be attached to three different types of such sides in G' . First, let v be a vertex with in-degree 2 and out-degree 0. If no leaf is attached in obtaining G from G' , then G is not a rooted leaf-labeled graph. Moreover, if at least two leaves are attached to G' , then S and S' have a common pendant subtree with at least two leaves and can be further reduced by applying the subtree reduction. Hence, G is obtained from G' by attaching exactly one leaf to v . Second, let $e = (u, v)$ and $e' = (u', v)$ be two edge sides such that v is a vertex side. Let x_1 be the unique leaf that is attached to v in obtaining G from G' . Now assume that at least two leaves x_2 and x_3 are attached to one of e and e' , say e . Without loss of generality, we may assume that (p_3, p_2) and (p_2, v) are edges in G , where p_2 and p_3 are the parent of x_2 and x_3 , respectively. Since $r(G) = r^\circ(S, S')$, it follows that, regardless of how many leaves are attached to e' , (x_1, x_2, x_3) is a pendant 3-chain in one of S and S' , and (x_2, x_3) is a pendant 2-chain in the other tree. This is because, if we consider subdivisions of S and S' in G , at least one of the two subdivisions does *not* use the edge (p_2, v) . If both used edge (p_2, v) , then the other edge entering v would not be used by either subdivision, and could safely be deleted, contradicting the assumed minimality of G i.e. $r(G) = r^\circ(S, S')$. Consequently, S and S' can be further reduced by applying the 3-2-chain reduction. Hence G is obtained from G' by attaching at most one leaf to e and at most one leaf to e' . Third, let e be an edge side that is not directed into a vertex side. If at least four leaves are attached in obtaining G from G' , then S and S' have a common 4-chain and can be further reduced by the chain reduction. Hence G is obtained from G' by attaching at most three leaves to e . Now, in G' , let k_0 be the number of vertex sides, and let k_1 be the number of vertices with in-degree 2 and out-degree 1. Then $k = k_0 + k_1$. Moreover, by Lemma 4.2, G' has $4k_0 + 3k_1 - 1 = 2k_0 + 2k_0 + 3k_1 - 1$ edge sides. Since there are $2k_0$ edge sides that are directed into a vertex side and $2k_0 + 3k_1 - 1$ edge sides that are not directed into a vertex side, we have

$$\begin{aligned} |X| &\leq 1 \cdot 2k_0 + 3(2k_0 + 3k_1 - 1) + 1 \cdot k_0 \\ &= 9k_0 + 9k_1 - 3 = 9k - 3 = 9d_{\text{rSPR}}(S, S') - 3. \quad \square \end{aligned}$$

We next establish that the bound as stated in the last theorem is tight. The approach we take is similar to that of [11, Theorem 6]. We start by briefly introducing some new definitions and refer the interested reader to [11] (and references therein such as [1,6,14]) for full details. A *binary character* f on X is a function that assigns each element in X to an element in $\{0, 1\}$. Let T be an unrooted binary phylogenetic X -tree with vertex set V , that is, T can be obtained from a rooted binary phylogenetic X -tree (without ρ) by suppressing its root with in-degree

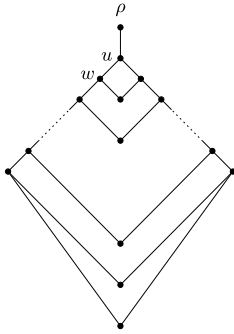


Fig. 3. For $k \geq 1$, the cyclic k -generator G'_k used in the construction of a family of pairs of rooted phylogenetic trees to show that the linear kernel established in Theorem 6.2 is tight. All edges are directed downwards.

0 and out-degree 2. An extension g of f to V is a function g that assigns each element in V to an element in $\{0, 1\}$ such that $g(x) = f(x)$ for each $x \in X$. The *parsimony score* of f on T , denoted by $l_f(T)$, denotes the minimum number of edges $\{u, v\}$ in T such that $g(u) \neq g(v)$, ranging over all extensions of f . Now, for two unrooted binary phylogenetic X -trees T and T' , the *maximum parsimony distance on binary characters* d^2_{MP} is defined as $d^2_{MP}(T, T') = \max_f |l_f(T) - l_f(T')|$ where f ranges over all binary characters on X . Lastly, the *tree bisection and reconnection distance* $d_{TBR}(T, T')$ between T and T' can, informally, be viewed as the minimum number of operations needed to transform T into T' , where each operation consists of deleting an edge in a tree and then re-attaching the two resulting (smaller) trees back together by joining them with a new edge. It is an unrooted analogue of the rSPR distance. Indeed, similar to Theorem 2.1, Allen and Steel [1] have shown that $d_{TBR}(T, T')$ can be characterized by (unrooted) maximum agreement forests. In what follows, the maximum parsimony distance on binary characters and the TBR distance between T and T' will play an important role because $d^2_{MP}(T, T')$ is a lower bound on $d_{TBR}(T, T')$ [6] and $d_{TBR}(T, T')$ is a lower bound on the rSPR distance between two rooted binary phylogenetic X -trees that can be obtained by rooting T and T' . We now make this more precise.

Theorem 6.3. *Let S and S' be two rooted phylogenetic X -trees such that $d_{rSPR}(S, S') \geq 1$. Suppose that S and S' cannot be reduced any further by applying the subtree, chain, or 3-2-chain reduction. Then $|X| \leq 9d_{rSPR}(S, S') - 3$ is a tight bound.*

Proof. Let $k \geq 1$, and let G'_k be the cyclic k -generator that is shown in Fig. 3. Observe that G'_k has k vertex sides, $2k$ edge sides that are directed into a vertex side and $2k - 1$ edge sides that are not directed into a vertex side. Obtain a rooted leaf-labeled graph G_k on $X \cup \{\rho\}$ from G'_k by attaching one leaf to each vertex side and to each edge side directed into a vertex side, and attaching three leaves to each remaining edge side. Then $|X| = k + 2k + 3(2k - 1) = 9k - 3$.

In what follows, we say that an edge (u, v) that is directed into a reticulation in G_k is a *left reticulation edge* (resp. *right reticulation edge*) if, in the process of obtaining G_k from G'_k , u subdivides an edge side (p, v) of G'_k ,

where v is a vertex side and p is to the left (resp. right) of v in Fig. 3. Now, let S_k be the rooted phylogenetic tree with label set $X \cup \{\rho\}$ obtained from G_k by deleting all right reticulation edges and suppressing all resulting vertices of in-degree 1 and out-degree 1. Similarly, let S'_k be the rooted phylogenetic X -tree obtained from G_k by deleting all left reticulation edges and suppressing all resulting vertices of in-degree 1 and out-degree 1. It is straightforward to check that S_k and S'_k cannot be reduced under the subtree, chain, or 3-2-chain reduction. We next show that $d_{rSPR}(S_k, S'_k) = k$. By construction, S_k and S'_k are displayed by G_k and, so $d_{rSPR}(S_k, S'_k) \leq k$. It remains to show that $d_{rSPR}(S_k, S'_k) \geq k$. The claim holds immediately when $k = 1$ because $S_k \neq S'_k$. Hence, we assume that $k \geq 2$. Let \bar{S}_k and \bar{S}'_k be the two unrooted binary phylogenetic X -trees obtained from S_k and S'_k , respectively, by deleting ρ , suppressing the resulting vertex of in-degree 0 and out-degree 2, and ignoring the directions on the edges. Consider the edge side (u, w) of G'_k as shown in Fig. 3. By construction, and because $k \geq 2$, there is a directed path $(u, v_1), (v_1, v_2), (v_2, v_3), (v_3, w)$ in G_k and, therefore, also in S_k . Now let f be the binary character that assigns 0 to each element in X if and only if it is a descendant of v_1 in S_k . Then $l_f(\bar{S}_k) = 1$. On the other hand, by applying the well-known Fitch algorithm [7], we see that $l_f(\bar{S}'_k) = k + 1$ and, thus,

$$1 - (k + 1) = k \leq d^2_{MP}(\bar{S}_k, \bar{S}'_k) \leq d_{TBR}(\bar{S}_k, \bar{S}'_k),$$

where the last inequality is established in [6]. We next show that $d_{TBR}(\bar{S}_k, \bar{S}'_k)$ is a lower bound on $d_{rSPR}(S_k, S'_k)$. Let F_k be a maximum agreement forest for S_k and S'_k . Let L_ρ be the element in F_k such that $\rho \in L_\rho$. Then, the forest \bar{F}_k obtained from F_k by replacing L_ρ with $L_\rho \setminus \{\rho\}$ is an (unrooted) agreement forest for \bar{S}_k and \bar{S}'_k with $|\bar{F}_k| \leq |F_k|$. In summary, we have

$$k \leq d^2_{MP}(\bar{S}_k, \bar{S}'_k) \leq d_{TBR}(\bar{S}_k, \bar{S}'_k) \leq |\bar{F}_k| - 1 \leq |F_k| - 1 = d_{rSPR}(S_k, S'_k), \tag{2}$$

where the third inequality follows from [1]. Setting $S = S_k$ and $S' = S'_k$, the theorem now follows. \square

7. Minimum hybridization

In this section, we turn to rooted leaf-labeled graphs without any directed cycle which are known as *rooted phylogenetic networks*. In this context, computing the *hybridization number*

$$r(T, T') = \min_N \{r(N)\},$$

where the minimum is taken over all rooted phylogenetic networks that display T and T' , has attracted much interest over the last 15 years. The hybridization number can also be characterized in terms of agreement forests. Let $F = \{L_\rho, L_1, \dots, L_k\}$ be an agreement forest for T and T' . Then F is *acyclic* if the graph G_F with vertex set F and for which (L_i, L_j) with $i, j \in \{\rho, 1, \dots, k\}$ is an edge precisely if

- (i) the root of $T[L_i]$ is an ancestor of the root of $T[L_j]$,
or
- (ii) the root of $T'[L_i]$ is an ancestor of the root of $T'[L_j]$

does not contain a directed cycle. Moreover, a *maximum acyclic agreement forest* for T and T' is an acyclic agreement forest for T and T' whose number of elements is minimum.

Theorem 7.1. [2] *Let T and T' be two rooted phylogenetic X -trees, and let F be a maximum acyclic agreement forest for T and T' . Then $r(T, T') = |F| - 1$.*

Computing $r(T, T')$ is known to be NP-hard but fixed-parameter tractable [4,5], and the current best weighted kernel has size at most $9k$, where $k = r(T, T')$ [13]. Viewed without weighting, the hybridization number kernel is quadratic in size [19]. This result relies on applying the subtree reduction and the following modified chain reduction that reduces a common n -chain to a (weighted) 2-chain, and k -generators which are cyclic k -generators with no directed cycle.

Chain reduction. For $n \geq 3$, let $C = (x_1, x_2, \dots, x_n)$ be a maximal n -chain that is common to T and T' . Then set $S = T|X \setminus \{x_3, x_4, \dots, x_n\}$ and $S' = T'|X \setminus \{x_3, x_4, \dots, x_n\}$.

It is natural to ask whether or not the 3-2-chain reduction can also be applied when computing $r(T, T')$. The next lemma answers this question affirmatively. A slightly more general result was also established in [20].

Lemma 7.2. *Let T and T' be two rooted phylogenetic X -trees, and let S and S' be two trees obtained from T and T' , respectively, by a single application of the 3-2-chain reduction. Then $r(S, S') = r(T, T') - 1$.*

Proof. This proof can be established in exactly the same way as the proof of Lemma 5.1 by replacing each occurrence of “agreement forest” with “acyclic agreement forest”, each occurrence of “ $d_{\text{rSPR}}(T, T')$ ” (resp. “ $d_{\text{rSPR}}(S, S')$ ”) with “ $r(T, T')$ ” (resp. “ $r(S, S')$ ”), and noting that the construction given in the proof of Lemma 5.1 results in an acyclic agreement forest. \square

Let T and T' be two rooted phylogenetic X -trees, and let S_1 and S'_1 be two trees resulting from T and T' , respectively, by exhaustively applying the subtree and chain reduction. In [4] a weight is associated to each 2-chain that results from applying the chain reduction. Without going into detail, a common n -chain is reduced to a 2-chain with a weight of, essentially, $n - 2$. The weights are necessary to compute the size of a maximum acyclic agreement forest for T and T' given such a forest for S_1 and S'_1 . Hence, if we first apply a chain reduction and, subsequently, a 3-2-chain reduction, we would need to take into account the weight of any previously reduced n -chain with $n \geq 3$. To avoid this, we establish the following.

Lemma 7.3. *Let T and T' be two rooted phylogenetic X -trees. Let S_2 and S'_2 be two trees obtained from T and T' , respectively, by applying the subtree and 3-2-chain reduction until no such*

reduction is possible, and let S and S' be two trees obtained from S_2 and S'_2 , respectively, by applying the chain reduction until no further reduction is possible. Then none of the three reductions can be applied to S and S' .

Proof. We make use of the following observations. First, the chain reduction cannot create new common pendant subtrees. Second, the chain reduction cannot use leaves from a weighted 2-chain created earlier since this would contradict the maximality of the chain that was reduced earlier. Hence, we can view exhaustive applications of the chain reduction as simultaneously applying the reduction to a maximal set of leaf-disjoint maximal common chains in S_2 and S'_2 , immediately yielding S and S' . Clearly, S and S' do not have a common subtree or n -chain with $n \geq 3$. Assume that S and S' can be further reduced under the 3-2-chain reduction. Then there exist a pendant 3-chain $C_3 = (x_1, x_2, x_3)$ in one of S or S' , say S , and a pendant 2-chain $C_2 = (x_3, x_i)$ with $i \in \{1, 2\}$ in S' . Since S_2 and S'_2 cannot be reduced any further under the 3-2-chain reduction, C_3 is not a pendant chain in S_2 or C_2 is not a pendant chain of S'_2 ; and the existence of C_1 and C_2 is necessarily caused by leaves that are deleted by the chain reduction. First, if C_2 is not pendant in S'_2 , then there exists a pendant 2-chain $c \in \{(x_i, x_j), (x_3, x_i)\}$ in S'_2 with $x_i \in X \setminus \{x_1, x_2, x_3\}$, and an n -chain C with $n \geq 3$ such that C is common to S_2 and S'_2 and the first two elements of C are identical with those of c . In obtaining S and S' from S_2 and S'_2 respectively, C is reduced to c ; thereby contradicting that C_2 is pendant in S' . Second, if C_3 is not pendant in S_2 , then an element $c \in \{(x_1, x_i), (x_2, x_i), (x_3, x_i), (x_1, x_2, x_i)\}$ is a pendant chain in S_2 . Moreover, similar to the first case there exists an n -chain C with $n \geq 3$ such that C is common to S_2 and S'_2 and the first two (resp. three) elements of C are identical with those in c . If $c \neq (x_1, x_2, x_i)$, then C is reduced to a 2-chain that contains x_i ; thereby contradicting that C_3 is pendant in S' . On the other hand, if $c = (x_1, x_2, x_i)$ then, as C is common to S_2 and S'_2 , it follows that (x_i, x_3, x_j) is a pendant 3-chain of S'_2 and (x_i, x_j) is a pendant 2-chain of S_2 , where x_j is the leaf in $\{x_1, x_2\}$ not equal to x_i . Hence S_2 and S'_2 can be reduced by a 3-2-chain reduction; a contradiction. \square

The next theorem establishes an improved kernel for computing $r(T, T')$.

Theorem 7.4. *Let S and S' be two rooted phylogenetic X -trees such that $r(S, S') \geq 1$. Suppose that S and S' cannot be reduced any further by applying the subtree, 3-2-chain, or chain reduction. Then $|X| \leq 7r(S, S') - 2$.*

Proof. Let G be a rooted phylogenetic network on X that displays S and S' such that $r(G) = r(S, S') = k \geq 1$, and let G' be the k -generator underlying G . Recall the chain reduction that is described at the start of Section 7. Then analogous to the proof of Theorem 6.2, G can be obtained from G' by attaching exactly one leaf to each vertex side, at most one leaf to each edge side that is directed into a vertex side, and at most two leaves to each edge side that is not directed into a vertex side. Now, let $k = k_0 + k_1$,

where k_0 is the number of vertex sides of G' and k_1 is the number of vertices with in-degree 2 and out-degree 1 in G' . Since Lemma 4.2 also applies to generators without any directed cycle, it follows that G' has $2k_0$ edges sides that are directed into a vertex side and $2k_0 + 3k_1 - 1$ edge sides that are not directed into a vertex side. Hence

$$\begin{aligned} |X| &\leq 1 \cdot 2k_0 + 2(2k_0 + 3k_1 - 1) + 1 \cdot k_0 \\ &= 7k_0 + 6k_1 - 2 \leq 7k - 2 = 7r(S, S') - 2. \quad \square \end{aligned}$$

As the next theorem shows, the kernel presented in the last theorem is again tight.

Theorem 7.5. *Let S and S' be two rooted phylogenetic X -trees such that $r(S, S') \geq 1$. Suppose that S and S' cannot be reduced any further by applying the subtree, 3-2-chain, or chain reduction. Then $|X| \leq 7r(S, S') - 2$ is a tight bound.*

Proof. First observe that the k -generator G'_k used in the proof of Theorem 6.3 is acyclic. Obtain a rooted phylogenetic network G_k on $X \cup \{\rho\}$ from G'_k by attaching one leaf to each vertex side and to each edge side directed into a vertex side, and attaching two leaves to each remaining edge side. Then $|X| = k + 2k + 2(2k - 1) = 7k - 2$. Since $d_{\text{rSPR}}(T, T') \leq r(T, T')$ for any two rooted phylogenetic trees, tightness can now be established in exactly the same way as in the second paragraph of the proof of Theorem 6.3 and replacing Inequality (2) with

$$\begin{aligned} k &\leq d_{\text{MP}}^2(\bar{S}_k, \bar{S}'_k) \leq d_{\text{TBR}}(\bar{S}_k, \bar{S}'_k) \\ &\leq |\bar{F}_k| - 1 \leq |F_k| - 1 = d_{\text{rSPR}}(S_k, S'_k) \leq r(S_k, S'_k). \quad \square \end{aligned}$$

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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