

The agreement distance of rooted phylogenetic networks

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The minimal number of rooted subtree prune and regraft (rSPR) operations needed to transform one phylogenetic tree into another one induces a metric on phylogenetic trees – the rSPR-distance. The rSPR-distance between two phylogenetic trees T and T' can be characterised by a maximum agreement forest; a forest with a minimum number of components that covers both T and T' . The rSPR operation has recently been generalised to phylogenetic networks with, among others, the subnetwork prune and regraft (SNPR) operation. Here, we introduce maximum agreement graphs as an explicit representations of differences of two phylogenetic networks, thus generalising maximum agreement forests. We show that maximum agreement graphs induce a metric on phylogenetic networks – the agreement distance. While this metric does not characterise the distances induced by SNPR and other generalisations of rSPR, we prove that it still bounds these distances with constant factors.

Keywords: phylogenetic network, rSPR, prune and regraft, maximum agreement forest, agreement distance

1 Introduction

A *phylogenetic tree* is a tree with its leaves labelled by a set of taxa; for example a set of organisms, species or languages (Semple and Steel, 2003; Dunn, 2014). Phylogenetic trees are used to visualise and study the inferred evolutionary history of such taxa. A *phylogenetic network* is a graph with its leaves labelled by a set of taxa, thus generalising a phylogenetic tree. While a phylogenetic tree models only bifurcating events, a phylogenetic network can also model reticulation events like hybridisation, recombination and horizontal gene transfer (Huson et al., 2010). The phylogenetic trees and networks considered here are all rooted and binary, i.e., they are directed acyclic graphs and all their vertices except their roots and leaves have degree three.

A tree rearrangement operation transforms one phylogenetic tree into another via a local graph-based change. For example, the *rooted subtree prune and regraft* (rSPR) operation prunes (cuts) a subtree of a phylogenetic tree and then regrafts (attaches) it to an edge of the remaining tree, resulting in another phylogenetic tree. See Figure 1 for an example. The minimal number of rSPR operations needed to transform one phylogenetic tree into another defines the rSPR-distance, which is a metric on the set of phylogenetic

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trees (Bordewich and Semple, 2005). The problem of computing the rSPR-distance of two phylogenetic trees is known to be NP-hard, but fixed-parameter tractable in its natural parameter (Bordewich and Semple, 2005). Moreover, the rSPR-distance induces the notion of neighbourhoods and thus organises the set of phylogenetic trees into a space. This is important in local search and MCMC algorithms that compute optimal phylogenetic trees (Felsenstein, 2004; St. John, 2017).

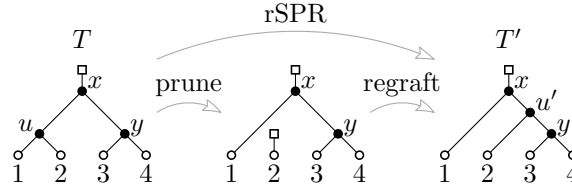


Fig. 1: An rSPR operation that transforms T into T' by first pruning the edge $(u, 2)$ at u and then regrafting it to the edge (x, y) . This process suppresses the vertex u and creates a new vertex u' that subdivides the edge (x, y) .

An rSPR-sequence that transforms one tree into another tree describes a series of prunings. The subtrees unchanged by the sequence form an *agreement forest* for these two trees. In other words, an agreement forest is the set of trees on which the two trees “agree” upon and that if put together cover each tree. See Figure 2 for an example. A *maximum agreement forest* (one that has a minimum number of trees) for two phylogenetic trees characterises their rSPR-distance (Bordewich and Semple, 2005). This means that in order to compute or reason about the rSPR-distance it suffices to consider one static structure, a maximum agreement forest, instead of a shortest rSPR-sequence. The notion of maximum agreement forests has proven to be the underpinning concept for almost all theoretical results as well as practical algorithms that are related to computing the rSPR-distance (Bordewich and Semple, 2005; Bordewich et al., 2008; Wu, 2009; Bonet and St. John, 2009; Whidden et al., 2013; Chen et al., 2015; Bordewich et al., 2017b).

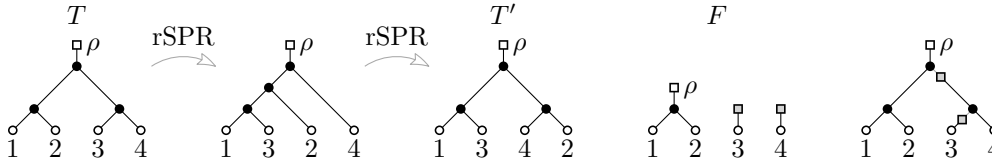


Fig. 2: An rSPR-sequence of length two that transforms T into T' , an agreement forest F for T and T' , and on the right how F covers T .

The rSPR operation was recently generalised to network rearrangement operations for phylogenetic networks (Bordewich et al., 2017a; Gambette et al., 2017). These generalisations have been studied in terms of computational complexity, shortest sequences and neighbourhoods (Bordewich et al., 2017a; Gambette et al., 2017; Janssen et al., 2018; Francis et al., 2018; Klawitter, 2018; Klawitter and Linz, 2019). Like rSPR these operations allow pruning and regrafting of edges. They add extra operations of adding and removing reticulations (vertices with in-degree two). It has to be distinguished whether edges can be pruned at their head and tail or only at their tail, and whether networks can contain parallel edges or not. Here, we allow parallel edges and consider the *subnetwork prune and regraft* (SNPR)

operation by Bordewich et al. (2017a), which only allows pruning at the tail, and the *prune and regraft* (PR) operation that also allows pruning at the head. Since computing the rSPR-distance between two phylogenetic trees is NP-hard (Bordewich et al., 2017a), it is not surprising that computing the distance of its generalisations is also NP-hard (Bordewich et al., 2017a; Gambette et al., 2017; Janssen et al., 2018). The study of shortest SNPR-sequences and PR-sequences has identified further difficulties for the computation of these distances (Klawitter and Linz, 2019). Together with the importance of agreement forests for the rSPR-distance, this motivates the questions of whether agreement forests are generalisable for rooted binary phylogenetic networks and, if so, whether they characterise the SNPR or PR-distance.

In this paper, we partially answer these two questions. First, with *(maximum) agreement graphs* we introduce a generalisation of (maximum) agreement forests for rooted binary phylogenetic networks (Section 3). Then we show that maximum agreement graphs induce a metric on phylogenetic networks, which we call the *agreement distance* (Section 4). While maximal agreement forests characterise the rSPR-distance, we show that this agreement distance does in general not equal the distance induced by a generalisation of rSPR. On the upside, we prove that the agreement distance bounds the PR-distance and the SNPR-distance from below naturally and from above with constant factors three and six, respectively (Section 5). We end this paper with some concluding remarks (Section 6).

2 Preliminaries

This section contains the definitions of rooted binary phylogenetic networks and trees, of network rearrangement operations and of their induced metrics. The definition of an agreement graph is given in the next section.

Phylogenetic networks and trees. Let $X = \{1, 2, \dots, n\}$ be a finite set. A *rooted binary phylogenetic network* N on X is a rooted directed acyclic graph with the vertices being

- the unique *root* labelled ρ with in-degree zero and out-degree one,
- *leaves* with in-degree one and out-degree zero bijectively labelled with X ,
- *inner tree vertices* with in-degree one and out-degree two, and
- *reticulations* with in-degree two and out-degree one.

The *tree vertices* of N are the union of the inner tree vertices, the leaves and the root. An edge $e = (u, v)$ is called a *reticulation edge* if v is a reticulation. Following Bordewich et al. (2017a), edges in N can be in *parallel*, that is, two distinct edges join the same pair of vertices. For two vertices u and v in N , we say that u is a *parent* of v and v is a *child* of u if there is an edge (u, v) in N . Similarly, we say that u is an *ancestor* of v and v is a *descendant* of u if there is a directed path from u to v in N . An edge (u, v) is an *ancestor* of an edge (x, y) and a vertex x if $v = x$ or if v is an ancestor of x . In this case, (x, y) is a *descendant* of (u, v) and v . Note that a vertex or an edge cannot be its own ancestor or descendant.

A *rooted binary phylogenetic tree* on X is a rooted binary phylogenetic network that has no reticulations. To ease reading, we refer to a rooted binary phylogenetic network (resp. rooted binary phylogenetic tree) on X simply as a phylogenetic network or network (resp. phylogenetic tree or tree). Furthermore, let \mathcal{N}_n denote the set of all phylogenetic networks on X and let \mathcal{T}_n denote the set of all phylogenetic trees on X where $n = |X|$.

PR and SNPR. Let $N \in \mathcal{N}_n$ with root ρ and let $e = (u, v)$ be an edge of N . Then the *prune and regraft* (PR) operation is an operation that transforms N into a phylogenetic network $N' \in \mathcal{N}_n$ in one of the following four ways:

- (PR⁰) If u is a tree vertex (and $u \neq \rho$), then delete e , suppress u , subdivide an edge that is not a descendant of v with a new vertex u' , and add the edge (u', v) ; or if v is a reticulation, then delete e , suppress v , subdivide an edge that is not an ancestor of u with a new vertex v' , and add the edge (u, v') .
- (PR⁺) Subdivide (u, v) with a new vertex v' , subdivide an edge in the resulting graph that is not a descendant of v' with a new vertex u' , and add the edge (u', v') .
- (PR⁻) If u is a tree vertex and v is a reticulation, then delete e and suppress u and v .

As the name suggests, we understand a PR⁰ operation as the process of “pruning” the edge (u, v) and then “regrafting” it to the subdivision of another edge. We say that the PR⁰ *prunes* (u, v) at u if u is the vertex that gets suppressed and a new vertex u' gets added. A PR⁰ operation that prunes an edge (u, v) at its head vertex v (resp. tail vertex u) is called a *head (tail) PR⁰* operation. Note that PR⁰ operations do not change the number of reticulations, while PR⁻ decreases it by one and PR⁺ increases it by one. These operations are illustrated in Figure 3. Furthermore, note that the *head* and *tail moves* defined by Gambette et al. (2017) (and further studied by Janssen et al. (2018)) conceptually equal head and tail PR⁰, but are restricted to networks without parallel edges.

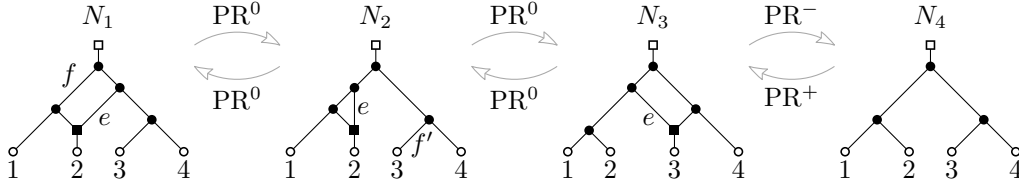


Fig. 3: The phylogenetic network N_2 (resp. N_3) can be obtained from N_1 (resp. N_2) by the tail PR⁰ (resp. head PR⁰) that prunes e and regrafts it to f (resp. f'). The phylogenetic network N_4 can be obtained from N_3 with the PR⁻ that removes e . Each operation has its corresponding PR⁰ and PR⁺ operation, respectively, that reverses the transformation.

The *subnet prune and regraft* (SNPR) operation by Bordewich et al. (2017a) equals the PR operation without head PR⁰. That is, an edge (u, v) can only be pruned at u , but not at v . Further note that the PR operation restricted to phylogenetic trees is the same as the well known rSPR operation. As Bordewich et al. (2017a) and Gambette et al. (2017) have shown, the different types of PR operations are all reversible. This means that for every PR⁰ (or SNPR⁰) that transforms N into N' there exists a PR⁰ (resp. SNPR⁰) that transforms N' into N , and that for every PR⁺ there exists an inverse PR⁻.

Distances. Let $N, N' \in \mathcal{N}_n$. A PR-*sequence* from N to N' is a sequence

$$\sigma = (N = N_0, N_1, N_2, \dots, N_k = N')$$

of phylogenetic networks such that, for each $i \in \{1, 2, \dots, k\}$, N_i can be obtained from N_{i-1} by a single PR. The *length* of σ is k . The PR-*distance* $d_{\text{PR}}(N, N')$ between N and N' is the length of a shortest

PR-sequence from N to N' . The SNPR-distance is defined analogously. Bordewich et al. (2017a) have shown that the SNPR-distance is a metric on \mathcal{N}_n . By the definition of the PR operation and its relation to the SNPR operation, it thus follows that the PR-distance is a metric on \mathcal{N}_n . Moreover, when restricted to \mathcal{T}_n , the SNPR- and the PR-distance equal the analogously defined rSPR-distance (Bordewich et al., 2017a).

3 Agreement graph

In this section, we define maximum agreement graphs for two phylogenetic networks N and N' . The main idea is to find a graph that can be obtained from both N and N' with a minimum number of prunings (as defined below). Throughout this section, let $N, N' \in \mathcal{N}_n$ with r and r' reticulations, respectively. Without loss of generality, assume that $r' \geq r$ and let $l = r' - r$ be the difference of the number of reticulations of N and N' . Furthermore, we assume that a path in a directed graph is a directed path and contains at least one edge.

Prunings and sprouts. In the last section, we have interpreted the pruning of an edge as half a step of a PR^0 operation (as the name prune and regraft suggests). We now extend this to a full operation that yields a new graph. Let G be a directed graph. Let u be a vertex of G that is either labelled or has degree three. Let (u, v) be an edge of G . Then a *pruning* of (u, v) at u is the process of deleting (u, v) and adding a new edge (\bar{u}, v) , where \bar{u} is a new (unlabelled) vertex. If u is now an in-degree one, out-degree one vertex, then suppress u . Note that a pruning does not remove a label from u . The definition for a pruning of the edge (u, v) at v is analogous. We mostly apply a pruning to a phylogenetic network or a graph derived from a phylogenetic network. Therefore, the restriction that u is either labelled or has degree three can be understood as u being either the root ρ , a (labelled) leaf, or an internal vertex.

A *sprout* of G is an unlabelled degree one vertex of G . For example, applying a pruning to a phylogenetic network yields a graph with exactly one sprout. A *t-sprout* (resp. *h-sprout*) is a sprout that is the tail (resp. head) of its incident edge.

Subdivisions and embeddings. Let G be a directed graph. An edge (u, v) of G is *subdivided* if (u, v) is replaced by a path from u to v . Recall that we assume that a path is a directed path containing at least one edge. A *subdivision* G^* of G is a graph that can be obtained from G by subdividing edges of G . Note that if G does not contain in-degree one, out-degree one vertices, then there exists a canonical mapping of vertices of G to vertices of G^* and of edges of G to paths of G^* .

Assume that G is connected. Then we say G has an *embedding* into N if there exists a subdivision G^* of G that is a subgraph of N . Now assume that G has components C_1, \dots, C_k . Then we say G has an *embedding* into N if the components C_i of G , for $i \in \{1, \dots, k\}$, have embeddings into N to pairwise edge-disjoint subgraphs of N . Note that these definitions imply that an embedding preserves the direction of edges of G^* into N and maps a labelled vertex of G^* to a vertex of N with the same label.

Agreement embeddings. Let (u, v) be an edge of N with u either a labelled vertex, i.e., the root ρ , or a degree-three vertex. Consider a graph G obtained from N by pruning (u, v) at u . Then G has exactly one sprout \bar{u} , and $n + 1$ labelled vertices of which n are bijectively labelled by X and one with ρ . We can distinguish three cases. If u is the labelled vertex ρ in N , then G contains an isolated labelled ρ , say, \bar{u}' . If u is a reticulation in N , then G contains an in-degree two, out-degree zero vertex, say, \bar{u}' . If u is an inner tree vertex in N , then u gets suppressed in the process of the pruning. In the first two cases, we get

a canonical embedding of G into N that is a bijection of the edges of G to the edges of N and a surjection of the vertices of G to the vertices of N . Only \bar{u} and \bar{u}' of G get mapped to u of N . In the third case, we obtain such an embedding for a subdivision of G (which reverses the suppression of u) into N . The case for pruning (u, v) at v is similar. Together the three cases motivate the following definition.

Let G be a directed graph. We say G has an *agreement embedding* into N if there exists an embedding of G into N with the following properties.

- An edge (\bar{u}, \bar{v}) of G is mapped to a path from a vertex u to a vertex v of N such that \bar{u} is mapped to u and \bar{v} is mapped to v .
- The edges of G are mapped to pairwise edge-disjoint paths of N that together cover all edges of N .
- At most two vertices of G are mapped to the same vertex of N . In this case, one of these two vertices of G is a sprout and the other is either a labelled isolated vertex, or an in-degree two, out-degree zero vertex, or an in-degree zero, out-degree two vertex.
- For each labelled vertex v of N , there exists exactly one vertex \bar{v} with the same label in G and \bar{v} is mapped to v .

Note that if G has an agreement embedding into N , then G has $n + 1$ labelled vertices of which n are bijectively labelled by X and one with ρ . Furthermore, note that to every inner tree vertex of N either a tree vertex, or a t-sprout, or an h-sprout and an out-degree two, in-degree zero vertex of G gets mapped. The situation is similar for reticulations, leafs and the root.

Lemma 3.1. *Let G be a directed graph and $N \in \mathcal{N}_n$.*

Then G has an agreement embedding into N if and only if G can be obtained from N by a sequence of prunings.

Proof: If G can be obtained from N by a sequence of prunings, then an agreement embedding of G into N follows naturally. So assume that G has an agreement embedding into N . Then G can be constructed from a sequence of prunings as follows. Assume that G contains a t-sprout \bar{u} . If \bar{u} is mapped to a vertex u and the edge (\bar{u}, \bar{v}) is mapped to the path from u to v in N , with w the child of u in this path, then prune the edge (u, w) at u . This covers either of the cases of when \bar{u} is mapped to ρ , or to the same reticulation to which a degree two vertex of G is mapped, or to a tree vertex of N that lies on a path to which an edge of G is mapped. In either case, applying this pruning also either creates the isolated vertex ρ , a degree two vertex, or suppresses a vertex, respectively. A pruning for an h-sprout works analogously. We can find such a pruning for each sprout of G . Now consider the case where we have identified that we want to prune the edge $e = (u, v)$ at u and the edge $f = (u, w)$ at w . Let p be the parent of u . If we now prune e at u , then the edges f and (p, u) are removed when suppressing u and a new edge $f' = (p, w)$ added. In the resulting graph, we cannot prune f , but instead now want to prune f' at w . Further note that since G has an agreement embedding into N , no two edges have to be pruned at the same vertex. Hence, we can apply one pruning after the other on the edges identified in N or on the edges they get extended to by preceding prunings. As noted, this does not only create the sprouts, but also the labelled, isolated vertices and degree-two vertices and shrinks the path of N to which edges of G get mapped to edges. Hence, this sequence of prunings results in G . □

Agreement graphs. Recall that we assume that N' has l more reticulations than N . Let G be a directed graph with connected components S_1, \dots, S_k and E_1, \dots, E_l , such that the E_1, \dots, E_l each consist of a single directed edge. Then G is an *agreement graph* for N and N' if

- G without E_1, \dots, E_l has an agreement embedding into N , and
- G has an agreement embedding into N' .

For such an agreement graph, we refer to each S_i as an *agreement subgraph* and to each E_j as a *disagreement edge*. A *maximum agreement graph* G for N and N' is an agreement graph for N and N' with a minimal number of sprouts. Figures 4 and 5 give two examples of maximum agreement graphs.

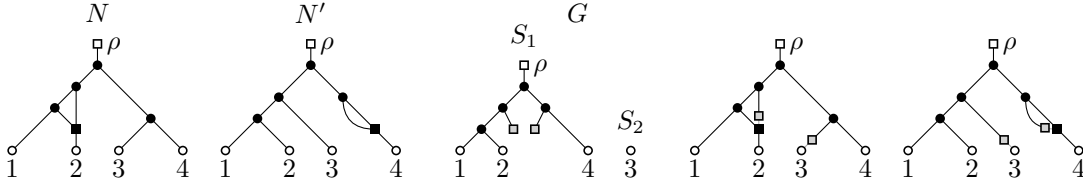


Fig. 4: A maximum agreement graph G for N and N' with its agreement embeddings into N and N' shown on the right. Note that the agreement subgraph S_2 consists of a labelled isolated vertex.

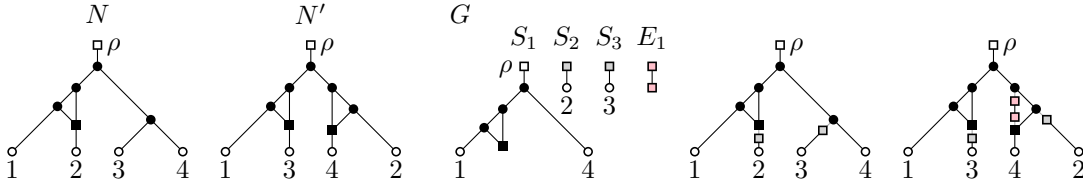


Fig. 5: A maximum agreement graph G for N and N' with its agreement embeddings into N and N' shown on the right. Note that the disagreement edge E_1 is only used for N' .

An *agreement forest* F for two trees T and T' is an agreement graph for T and T' where each agreement subgraph S_i for $i \in \{2, \dots, k\}$ is a phylogenetic tree with an unlabelled root and S_1 is either a phylogenetic tree (with the root labelled ρ) or an isolated vertex labelled ρ . Note that an agreement forest F contains no h-sprouts and that thus in the respective agreement embeddings of F into T and T' a sprout of F is mapped either to the root ρ or to a subdivision vertex of an edge of another agreement subgraph. See again Figure 2 for an example. On the other hand, considering shortest PR-sequences between N and N' in the examples in Figures 4 and 5 shows why in general in an agreement embedding of an agreement graph G a sprout may have to be mapped to the same vertex as a labelled isolated vertex (ρ or a leaf of N and N') or a non-suppressible degree-two vertex of G .

Before we show that maximum agreement graphs induce a metric on \mathcal{N}_n , we establish further notation and terminology to ease talking about agreement embeddings and agreement graphs. We use $\bar{e}, \bar{f}, \bar{u}, \bar{v}$ if we refer to edges or vertices of an agreement graph and e, f, u, v for edges and vertices of N or N' . If we use symbols like \bar{u} and u in the same context, then \bar{u} is usually mapped to u by the agreement embedding under consideration.

Let $G = (V_G, E_G)$ be a graph with an agreement embedding into a network $N = (V_N, E_N)$. We say a sprout $\bar{u} \in V_G$ is *attached* to $\bar{e} \in E_G$ in N if \bar{u} is mapped to a vertex $u \in V_N$ that is an internal vertex of the path to which \bar{e} is mapped. Similarly, we say $\bar{u} \in V_G$ is *attached* to $\bar{x} \in V_G$ in N if \bar{u} and \bar{x} are mapped to the same vertex $x \in V_N$. We say an edge $\bar{e} = (\bar{u}, \bar{v}) \in E_G$ is *attached* to $\bar{f} \in E_G$ in N if either \bar{u} or \bar{v} is a sprout and attached to \bar{f} . Note that \bar{e} being attached to \bar{f} does not imply \bar{f} being attached to \bar{e} . Considering the example in Figure 4 and the agreement embedding of G into N , note that one sprout is attached to the incoming edge of leaf 2 in N and another sprout is attached to the isolated vertex labelled 3 in N .

Embedding changes. Note that a graph G may have several agreement embeddings into N or N' . We now describe how, in some cases, an agreement embedding can be changed into another one. For this, let \bar{u} and \bar{v} be two t-sprouts of G with outgoing edges $\bar{e} = (\bar{u}, \bar{w})$ and $\bar{f} = (\bar{v}, \bar{z})$, respectively, such that \bar{u} is attached to \bar{f} in N . Let \bar{e} be mapped to the path $P = (y, \dots, w)$ in N and let \bar{f} be mapped to the path $P' = (x, \dots, y, \dots, z)$ in N . Then an *embedding change* of G into N with respect to \bar{u} and \bar{v} is the change of the embedding such that \bar{e} is mapped to the path (x, \dots, y, \dots, w) formed by a subpath of P' and the path P , and such that \bar{f} is mapped to the subpath (y, \dots, z) of P' . See Figure 6 for an example. The definition for h-sprouts is analogous.

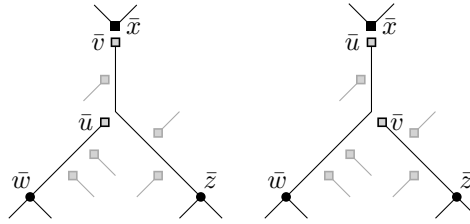


Fig. 6: An embedding change with respect to \bar{u} and \bar{v} .

We now use embedding changes to show that an agreement embedding of G into N' can be changed into an agreement embedding with some nice properties.

Lemma 3.2. *Let $N, N' \in \mathcal{N}_n$ with r and $r' > r$ reticulations, respectively. Let G be a maximum agreement graph for N and N' .*

Then there exist an agreement embedding of G into N' such that

- *no sprout of an agreement subgraph is attached to a disagreement edge, and*
- *at least one disagreement edge is not attached to any other disagreement edge, and*
- *a disagreement edge E_i of G may only be attached to a disagreement edge E_j of G if $j < i$.*

Proof: Fix an agreement embedding of G into N' . Assume that this embedding does not fulfill the first property. Then let \bar{u} be a sprout of an agreement subgraph of G that is attached to a disagreement edge (\bar{v}, \bar{w}) in N' . Without loss of generality, assume that \bar{u} is a t-sprout. Apply an embedding change with respect to \bar{u} and \bar{v} . If \bar{v} was attached to another disagreement edge (\bar{x}, \bar{y}) in N' , then repeat this step with \bar{u} and \bar{x} . Otherwise \bar{u} is now attached to a vertex or an edge of an agreement subgraph. This process

terminates since the vertex u to which \bar{u} gets mapped gets closer to the root in N' with every step. Note that the embedding change of \bar{u} and \bar{v} may cause a sprout \bar{z} that was previously attached to (\bar{v}, \bar{w}) in N' to now be attached to the edge incident to \bar{u} in N' . However, since this edge is an edge of an agreement subgraph, this does not negatively effect the first property. Therefore, every sprout that was previously attached to an edge of an agreement subgraph is still so after each step. Hence, each sprout \bar{u} of an agreement subgraph can be handled after the other and without negatively affecting property three.

Next, assume that the current embedding fulfills the first, but not the third property. Let $E_i = (\bar{u}, \bar{v})$ be a disagreement edge of G , starting with $E_i = E_1$. If \bar{u} and \bar{v} are each attached to a vertex or an edge of an agreement subgraph or to a disagreement edge E_j with $j < i$ in N' , then proceed with E_{i+1} . Otherwise, without loss of generality, assume that \bar{u} is attached to a disagreement edge $E_j = (\bar{x}, \bar{y})$ with $j > i$. Apply an embedding change with respect to \bar{u} and \bar{x} . The same arguments as above show that eventually \bar{u} is attached in N' in a good way. Since the embedding change does not affect a sprout of any E_m with $m < i$ or of an agreement subgraph, this process does not affect the first property or the previously handled disagreement edges. Therefore, each E_i can be handled after the other. Apply analogous steps, if necessary, to \bar{v} before proceeding with E_{i+1} . The process terminates after $E_i = E_l$ has been handled. Finally, note that the third property implies the second. \square

Next, we show how to prune a particular edge of G such that the resulting graph is still an agreement graph for N and N' .

Lemma 3.3. *Let $N, N' \in \mathcal{N}_n$. Let G be an agreement graph for N and N' . Let $\bar{e} = (\bar{u}, \bar{v})$ be an edge of G . Then G can be transformed into a graph G' such that*

- \bar{u} (or \bar{v}) is a sprout in G' ,
- G' contains at most one sprout more than G , and
- G' is an agreement graph for N and N' .

Proof: We prove this for a t-sprout \bar{u} . The proof for an h-sprout works analogously. If \bar{u} is already a sprout, then there is nothing to do. If \bar{u} is labelled ρ or \bar{u} has degree three, then obtain G' by pruning the edge \bar{e} at \bar{u} . So assume that \bar{u} is an in-degree zero, out-degree two vertex. Consider the agreement embedding of G into N . Let \bar{u} be mapped to u in N . Since u has degree three in N , there is an h-sprout \bar{w} mapped to u in N . This and the following process are illustrated in Figure 7. Then identify \bar{w} with \bar{u} , i.e., regraft \bar{w} to \bar{u} , and then prune \bar{e} from \bar{u} . Let G'' be the resulting graph. In the agreement embedding of the resulting graph into N , the new sprout \bar{u} is now attached to an edge $\bar{f} = (\bar{x}, \bar{y})$. To get \bar{w} back, restart this case distinction with the goal to prune \bar{f} at \bar{y} . Note that this process terminates since the number of degree two vertices in G'' is one less than in G and thus at some point one of the first two cases has to apply. Let G' be the resulting graph when the process has terminated. Then G' contains the sprout \bar{u} with incident edge \bar{e} and contains at most one sprout more than G . That is because before the case distinction got restarted, the sprout \bar{w} got removed first. Clearly, G' has an agreement embedding into N . If one of the first two cases applied, then it is also easy to show that G' has an agreement embedding into N' . Otherwise, note that in the agreement embedding of G into N' an h-sprout \bar{w}' is attached to the degree-two vertex \bar{u} . For the agreement embedding of G' into N' , this sprout \bar{w}' extends the same way as \bar{w} got extended in the embedding into N (see again Figure 7). \square

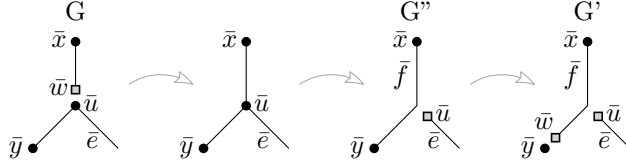


Fig. 7: For the proof of Lemma 3.3, how to prune the edge \bar{e} at a degree-two vertex \bar{u} . First, regraft \bar{w} ; second, prune \bar{e} at \bar{u} ; third, reobtain the sprout \bar{w} .

4 Agreement distance

The importance of the notion of maximum agreement forests lies in the fact that it defines a metric on \mathcal{T}_n that equals the rSPR-distance. In this section, we show that maximum agreement graphs similarly induce a metric on \mathcal{N}_n . Furthermore, we prove that this metric, if restricted to \mathcal{T}_n , also equals the rSPR-distance and is thus NP-hard to compute.

Let $N, N' \in \mathcal{N}_n$ and let l be the difference in number of reticulations of N and N' . Let G be a maximum agreement graph for N and N' with l disagreement edges. Let s be the total number of sprouts in the agreement subgraphs of G . Then define the *agreement distance* d_{AD} of N and N' as

$$d_{AD}(N, N') = s + l.$$

This is well defined since l is fixed by N and N' , and since s is minimal over all agreement graphs for N and N' by the choice of G .

Theorem 4.1. *The agreement distance d_{AD} on \mathcal{N}_n is a metric.*

Proof: We have to show that d_{AD} is symmetric, non-negative, that for all $M, M' \in \mathcal{N}_n$ $d_{AD}(M, M') = 0$ if and only if $M = M'$, and that d_{AD} satisfies the triangle inequality. Let N, N' , and l be as above. First note that the agreement distance is symmetric and non-negative by definition. Second, if $N = N'$, then $G = N$ is a maximum agreement graph for N and N' with zero sprouts and zero disagreement edges and thus $d_{AD}(N, N) = 0$. Now let G be a maximum agreement graph for N and N' with zero sprouts and zero disagreement edges, i.e., $d_{AD}(N, N') = 0$. Together with the fact that N and N' are internally binary, this implies that every unlabelled vertex of N and N' , respectively, gets covered by a degree three vertex of G . Thus G has to consist of a single connected component and has an agreement embedding into both N and N' without subdivisions. This in turn implies that $N = G = N'$.

Next, we prove that the agreement distance satisfies the triangle inequality. For this let $N, N', N'' \in \mathcal{N}_n$ with r, r' and r'' reticulations, respectively. With out loss of generality, assume that $r \leq r''$. Let G' (resp. G'') be a maximum agreement graph for N and N' (resp. N' and N'') with s' sprouts in its agreement subgraphs and l' disagreement edges (resp. s'' and l''). For the triangle inequality to hold, we have to show that

$$d_{AD}(N, N'') \leq d = d_{AD}(N, N') + d_{AD}(N', N'') = s' + s'' + l' + l''.$$

For this, we construct an agreement graph G for N and N'' with s sprouts in its agreement subgraphs and l disagreement edges such that $s + l \leq d$. Note that G does not have to be a maximum agreement graph. Also note that l is fixed by N and N'' . The main idea for the construction of G is to merge G' and G'' in terms of the prunings they represent in N, N' and N'' . Containing, so to say, sprouts from both G' and

G'' and the right amount of disagreement edges, finding agreement embeddings of G into N and N'' will become easy. We first consider the restricted cases of when N , N' and N'' either have the same number of reticulations or only differ in the number of reticulations.

Case I – $l' = l'' = 0$. In this case, by Lemma 3.1 both G' and G'' can be obtained from N' by applying s' and s'' prunings, respectively. We now apply all these prunings to N' to construct G in the following way. Like in Lemma 3.1, we identify to which edges of N' these prunings correspond and whether they prune at the tail or the head of the edge. Apply the s' prunings of G' to N' to obtain, of course, G' . Next, to apply the s'' prunings (in N') of G'' to G' , we have to identify which edges to prune in G' .

Assume, without loss of generality, that we want to prune $e = (u, v)$ at u in N' . Further assume G' contains an edge $\bar{e} = (\bar{u}, \bar{y})$ such that \bar{u} is mapped to u and \bar{e} to a path containing e . With Lemma 3.3 prune \bar{e} at \bar{u} and obtain a graph \bar{G} . Note that \bar{G} has an agreement embedding into N and N' . Next, assume G' contains an edge $\bar{e}' = (\bar{x}, \bar{y})$ such that \bar{e}' is mapped to a path containing e and u as internal vertex. Then, G' contains a sprout \bar{w} that is mapped to u (and thus attached to \bar{e}' in N'). If \bar{w} is an h-sprout, prune \bar{e}' at \bar{x} with Lemma 3.3 and obtain a graph \bar{G} . Note that \bar{G} has an agreement embedding into N and N' . So assume otherwise, namely that \bar{w} is a t-sprout. Let \bar{w} have the incident edge (\bar{w}, \bar{z}) . Subdivide \bar{e}' with a new vertex \bar{u} and identify \bar{w} with \bar{u} . Prune $\bar{e} = (\bar{u}, \bar{y})$ at \bar{u} and then use Lemma 3.3 to prune (\bar{x}, \bar{z}) at \bar{x} to reobtain \bar{w} . Let \bar{G} be the resulting graph. Note that \bar{G} has an agreement embedding into N' . Furthermore, apply an embedding change with respect to \bar{u} and \bar{w} to see that G still has an agreement embedding into N . Repeat this process (now using \bar{G} instead of G') for each of the s'' sprouts of G'' . Let G be the resulting graph, which by construction has an agreement embedding into N' and N . Furthermore, G has at most $s \leq s' + s''$ sprouts.

Lastly, we have to show that G has an agreement embedding into N'' . Consider the agreement embeddings of G and G'' into N' . Let \bar{u} be a sprout of G obtained for a sprout \bar{u}'' of G'' . If \bar{u} and \bar{u}'' are mapped to the same vertex u of N'' , then it is straightforward to handle \bar{u} when obtaining the agreement embedding of G into N'' . On the other hand, \bar{u} could “reach beyond” u , that is, its incident edge is mapped to a path containing u as internal vertex. This case might be reduced to the former with an embedding change of G into N' . Otherwise, we know that \bar{u}'' is attached to a degree two vertex \bar{x}'' in N' . Furthermore, there is then also a sprout \bar{w}'' of G'' that is attached to \bar{x}'' in the agreement embedding of G'' into N'' . Let \bar{w} be the sprout of G obtained for the sprout \bar{w}'' . Using the agreement embedding of G'' into N'' to obtain the agreement embedding of G into N'' , we then let the sprout \bar{w} “reach beyond” \bar{x}'' in the same way as \bar{u} does in the agreement embedding of G into N' (see also Figure 7). To conclude, note that with

$$s + l = s \leq s' + s'' = s' + s'' + l' + l''$$

the triangle inequality holds in this case.

Case II.a – $s' = s'' = 0$ and $r < r' < r''$. In this case, N' can be seen as N plus l' reticulation edges and N'' can be seen as N' plus l'' reticulation edges. Thus, N'' can also be seen as N plus $l' + l''$ reticulation edges. Therefore G consisting of N and $l = l' + l''$ disagreement edges is a desired agreement graph for N and N'' showing that the triangle inequality holds in this case.

Case II.b – $s' = s'' = 0$ and $r < r' > r''$. Fix agreement embeddings of G' and G'' into N' . Colour all edges to which a disagreement edge of G' is mapped orange and to which a disagreement edge of G'' is mapped green. Intuitively, edges that are now both green and orange in N' are neither in N nor in N'' . We now align the agreement embeddings of G' (and G'') such that a disagreement edge is mapped to either edges that are all orange or all green-orange (resp. all green or all green-orange). Note that a disagreement edge is mapped to a path that starts at a tree vertex and ends at a reticulation. Furthermore, if such a path

contains an internal vertex v , then the sprout of another disagreement edge is mapped to v . Therefore, to align the agreement embeddings as described above, we can apply a sequence of simple embedding changes to the sprouts of disagreement edges as illustrated in Figure 8 (i) and (ii) (the rules for h-sprouts and swapped colours are analogous). We can further align those disagreement edges of G' and G'' that are mapped to green-orange edges with rule (iii) in Figure 8. Now let k' be the number disagreement edges of G' (and thus also of G'') that are mapped to green-orange edges.

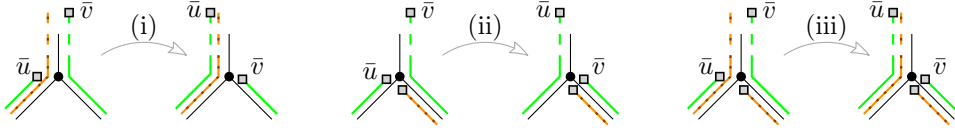


Fig. 8: For Case II.b, embedding changes of G'' (green) into N' with respect to \bar{u} and \bar{v} to align the embeddings of disagreement edges of G' (orange with dots) and G'' in N' .

Obtain a new N' from N' by removing all green-orange edges from N' , obtain new G' and G'' from G' and G'' by removing k' disagreement edges. Note that G'' has now $k = l'' - k'$ disagreement edges. Clearly, G' (resp. G'') has still an agreement embedding into N and N' (resp. N' and N''). Then, in N' , if a vertex is incident to an uncoloured edge e , an orange edge, and a green edge, then colour e red. Such a colouring is illustrated in Figure 9. Next and as long as possible, while a vertex is incident to an uncoloured edge e , a red edge and a green or orange edge, colour e red. Obtain S from N' by removing all coloured edges and suppressing in-degree one, out-degree one vertices. Removing the red edges prevents S from having sprouts. Let G be the graph consisting of S and l disagreement edges and $k = l'' - k'$ connected components F_i consisting of a single directed edge. We claim that G is an agreement graph for N and N'' .

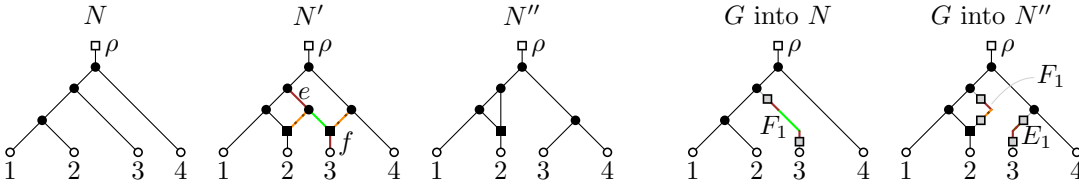


Fig. 9: For Case II.b, N (resp. N'') can be obtained from N' by removing the orange (with dots) (resp. green) edges. Embedding G into N , the agreement subgraph F_1 has to cover not only the green edge, but also the red edges (e and f), which got removed from N' when obtaining G because a disagreement edge of both N and of N'' were incident to them.

We construct an agreement embedding of G into N . The embedding of S into N is given by the embeddings of S and N into N' . Let E_i be a disagreement edge of G'' . Let P be the green path in N' that corresponds to E_i . If an edge of P caused the creation of a red edge e , extend P by e if possible, i.e., if P would still be a directed path. Next and as long as possible, if e caused another red edge e' , extend P by e' if possible. Then embed an F_i into N in the way that P is embedded onto N in the embedding of N into N' . The colours of the edges ensure that this is possible. See again Figure 9 for an example. Furthermore, note that this construction eventually covers all green and red edges. Hence, we constructed

an agreement embedding of G into N . Finding an agreement embedding of G into N'' works analogously but also uses the disagreement edges of G besides the F_i . Since $l = l' - l''$, we get

$$s + l = 2k + l \leq 2l'' + l = l' + l'',$$

and thus the triangle inequality also holds in this case.

Case II.c – $s' = s'' = 0$ and $r > r' < r''$. In this case, N and N'' can be obtained from N' by adding l' and $l'' = l + l'$ reticulation edges, respectively. Consequently, N' together with l disagreement edges and l' further connected components that consists of a single directed edge gives an agreement graph for N and N'' . Since $l = l'' - l'$, we get $s + l = 2l' + l = l' + l''$, and thus the triangle inequality also holds in this case.

Case III.a – $r \leq r' \leq r''$. Assume agreement embeddings of G' and G'' with nice properties as in Lemma 3.2. We now combine Case I and Case II.b to obtain G . Let H be the graph G'' without its disagreement edges. Note that H has an agreement embedding into N' and has s'' sprouts. Like in Case I, obtain a graph R from H by applying s' prunings in the way the s' sprouts of G' are attached to vertices in N' . Note that R has an agreement embedding into N' and has at most $s' + s''$ sprouts. Then like in Case II.b, obtain a graph S from R by removing all paths from R to which disagreement edges of G' are mapped. Again, handle conflicts between a sprout of a disagreement edge of G' and a sprout of R like the red edges in Case II.b. Now let G be the graph consisting of S and $l = l' + l''$ disagreement edges. Note that S and thus G have at most $s' + s''$ sprouts (ignoring those in the disagreement edges). Hence, $s + l \leq d$. Constructing agreement embeddings of G works again by combining the mechanisms from Case I and Case II.b.

The two cases for when $r \leq r' \geq r''$ and $r \geq r' \leq r''$ can be handled similarly to Case III.a together with the ideas from Case II.b and Case II.c. We give a brief outline of how G can be constructed.

Case III.b – $r \leq r' \geq r''$. Let S be the graph obtained from N' by removing all paths to which the disagreement edges of G' and G'' are mapped (like in Case II.b) and by applying the prunings of G' and G'' in the way they embed into N' (like in Case I). Again, in this process we have to take care of cases where two sprouts are mapped to the same vertex. Then the graph G consisting of S and $k \leq l''$ additional directed edges and l disagreement edges is an agreement graph for N and N'' with at most $s' + s'' + 2l''$ sprouts in agreement subgraphs and $l = l' - l''$ disagreement edges. Hence, $s + l \leq d$.

Case III.c – $r \geq r' \leq r''$. Let S be the graph obtained from N' by applying the prunings of G' and G'' in the way they embed into N' (like in Case I). Then the graph G consisting of S and l' additional directed edges and l disagreement edges is an agreement graph for N and N'' with at most $s' + s'' + 2l'$ sprouts in agreement subgraphs and $l = l'' - l'$ disagreement edges. Hence, $s + l \leq d$.

This concludes the proof. \square

Next, we show that if we restrict the agreement distance to the space of phylogenetic trees, then it equals the rSPR-distance.

Proposition 4.2. *The agreement distance on \mathcal{T}_n is equivalent to the rSPR-distance.*

Proof: Let $T, T' \in \mathcal{T}_n$. Let G be a maximum agreement graph for T and T' with components S_1, \dots, S_m . We distinguish whether G contains an h-sprout or not.

Assume G does not contain an h-sprout. Then G is a maximum agreement forest for T and T' . Therefore, $d_{AD}(T, T') = m - 1$, that is, it equals the number of components of G minus one. Furthermore, by removing sprouts and their incident edges from G we obtain a forest F that is a maximum agreement

forest for T and T' under the definition of Bordewich and Semple (2005). Hence, the statement follows from Theorem 2.1 by Bordewich and Semple (2005).

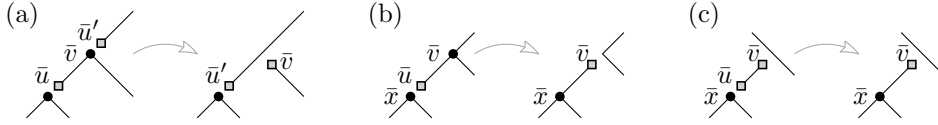


Fig. 10: How to convert h-sprouts from a maximum agreement graph G for two trees to t-sprouts for Proposition 4.2, when the h-sprout \bar{u} is child of a degree two vertex (a), a degree-three vertex (b), or a t-sprout (c), respectively.

Now assume G contains k h-sprouts. We now show how to derive a maximum agreement graph G' for T and T' without h-sprouts. Assume that G contains an h-sprout \bar{u} that is a child of a degree two vertex \bar{v} . Note that in the agreement embedding of G into T and T' there is another h-sprout attached to \bar{v} . Thus, deleting (\bar{u}, \bar{v}) from G creates a new t-sprout \bar{v} such that G is still a maximum agreement graph for T and T' (see Figure 10 (a)). So assume that G contains no such h-sprout. Hence, G contains k h-sprouts that are adjacent to degree three vertices, to ρ or a t-sprout. Then since a tree does not contain reticulations, note that G also contains k vertices with in-degree zero but out-degree either zero (a labelled leaf of T) or two. That is because in the agreement embedding of G into T and T' the k h-sprouts have to get mapped to such k vertices. Let M be the set of those vertices. Now, firstly, remove from G the k h-sprouts and their incident edges and suppress resulting degree two vertices. If this results in an unlabelled, isolated vertex, remove it too. This does not create any new sprouts since by assumption no h-sprout was incident to a degree two vertex. Secondly, add k edges connecting each vertex in M with a new t-sprout (see Figure 10 (b) and (c)). Let G' be the resulting graph. Note that G' contains either the same number of sprouts as G or less if an h-sprout was adjacent to a t-sprout in G . (Note that G was actually not a maximum agreement graph if the latter case applies.) Figure 10 also shows how to derive the agreement embeddings of G' into T and T' from the agreement embeddings of G . Hence G' is a maximum agreement graph for T and T' without h-sprouts and the claim follows from the previous case. \square

Bordewich and Semple (2005, Theorem 2.2) have shown that computing the rSPR-distance of two phylogenetic trees is NP-hard. Together with Proposition 4.2 this implies the following corollary.

Corollary 4.3. *Computing the agreement distance is NP-hard.*

5 Bounds on rearrangement distances

After we have shown that the agreement distance equals the rSPR-distance on \mathcal{T}_n , we now consider its relation to the PR- and SNPR-distance on \mathcal{N}_n . We start on a positive note concerning the neighbourhoods of a phylogenetic network under PR and the agreement distance.

Lemma 5.1. *Let $N, N' \in \mathcal{N}_n$. Then $d_{AD}(N, N') = 1$ if and only if $d_{PR}(N, N') = 1$.*

Proof: Assume $d_{PR}(N, N') = 1$. Depending on whether N' can be obtained from N by applying a PR^0 or a PR^+ operation, obtain a maximum agreement graph G by either mimicking the pruning or adding a disagreement edge to N . In either case, it follows that $d_{AD}(N, N') = 1$.

Now assume $d_{AD}(N, N') = 1$ and let G be a maximum agreement graph for N and N' . If G contains a disagreement edge, then it is easy to see that $d_{PR}(N, N') = 1$. So assume G contains a single sprout \bar{u} . If

\bar{u} is attached to a vertex \bar{x} of G in the agreement embedding into N , then it has to be attached to \bar{x} also in the agreement embedding into N' . However, then $N = N'$, which is a contradiction to $d_{AD}(N, N') = 1$. If, on the other hand, \bar{u} is attached to an edge of G in the agreement embedding into N (and thus into N'), then finding a PR^0 that transforms N into N' is straightforward. It follows that $d_{PR}(N, N') = 1$. \square

Consider the two networks N and N' shown in Figure 11. Observe that $d_{PR}(N, N') = 4$, but that $d_{AD}(N, N') = 3$ (which can both be shown with an exhaustive search). Intuitively, the differences arises from the fact that no PR^0 can prune, from N or N' , any of the three sprouts of the shown maximum agreement graph G and regraft it without creating a directed cycle. Nor is there a shortest PR-sequence of length three that uses PR^+ and PR^- operations. This shows that, in general, the agreement distance and the PR-distance differ on \mathcal{N}_n . Since allowing only tail PR^0 like SNPR does or not allowing parallel edges increases the distance in general, it follows that the agreement distances also differs from the SNPR-distance and distances of other generalisations of rSPR. Furthermore, there exist pairs of phylogenetic networks with $r \geq 1$ reticulations for which every shortest PR- or SNPR-sequence contains a phylogenetic tree (Klawitter and Linz, 2019). This implies that along such a sequence reticulation edges get removed and added again. Therefore, and even if the PR-distance (or SNPR-distance) and the agreement distance would be the same for such a pair, an agreement graph can in general not fully model every shortest PR- and SNPR-sequence. On the upside, however, we prove now that the agreement distance gives a lower and upper bound for the PR-distance with constant factors. We start with the lower bound.

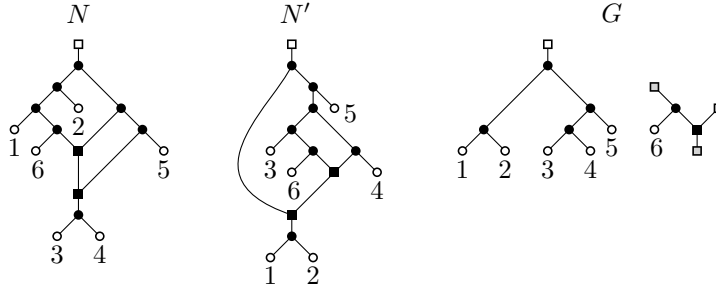


Fig. 11: Two phylogenetic networks N and N' with $d_{PR}(N, N') = 4$, but $d_{AD}(N, N') = 3$ as the maximum agreement graph G shows.

Theorem 5.2. *Let $N, N' \in \mathcal{N}_n$. Then $d_{AD}(N, N') \leq d_{PR}(N, N')$.*

Proof: Given N and N' with PR-distance $d = d_{PR}(N, N')$, we construct an agreement graph G of N and N' with s sprouts in the agreement subgraphs and l disagreement edges such that $s + l \leq d$. Let N and N' have r and r' reticulations, respectively. Without loss of generality, assume that $r' \geq r$ and let $l = r' - r$. The proof is now by induction on d . If $d = 0$, then $G = N$ is as desired. If $d = 1$, the statement follows from Lemma 5.1. Now assume that for each pair of phylogenetic networks $M, M' \in \mathcal{N}_n$ with PR-distance at most $d' < d$ for some arbitrary but fixed $d > 1$ there exists an agreement graph of M and M' proving that $d_{AD}(M, M') \leq d'$.

Fix a PR-sequence of length d from N to N' . Let $N'' \in \mathcal{N}_n$ be the network of that sequence such that $d_{PR}(N, N'') = d - 1$ and $d_{PR}(N'', N') = 1$. By the induction hypothesis there exists an agreement graph

G' for N and N'' showing that $d_{\text{AD}}(N, N'') \leq d - 1$. We distinguish whether N' is obtained from N'' by a PR^0 , a PR^+ , or a PR^- operation.

First, assume that N' can be obtained from N'' by pruning the edge $e = (u, v)$ at u . Assume G' contains an edge $\bar{e} = (\bar{u}, \bar{y})$ such that \bar{u} is mapped to u and \bar{e} to a path containing e . With Lemma 3.3 prune \bar{e} at \bar{u} and obtain G . Then use the agreement embedding of G into N'' to obtain an agreement embedding of G into N' . Next, assume G' contains an edge $\bar{e}' = (\bar{x}, \bar{y})$ such that \bar{e}' is mapped to a path containing e and u as internal vertex. Then, G' contains a t-sprout \bar{w} that is mapped to u (and thus attached to \bar{e}' in N''). The vertex \bar{w} cannot be an h-sprout, because u is a tree vertex and the previous case does not apply. Let \bar{w} have the incident edge (\bar{w}, \bar{z}) . Subdivide \bar{e}' with a new vertex \bar{u} and identify \bar{w} with \bar{u} . Prune $\bar{e} = (\bar{u}, \bar{y})$ at \bar{u} and then use Lemma 3.3 to prune (\bar{x}, \bar{z}) at \bar{x} to reobtain \bar{w} . Let G be the resulting graph, which has now an agreement embedding into N' . Considering the embedding of G into N'' , apply an embedding change with respect to \bar{u} and \bar{w} to see that G still has an agreement embedding into N . In either case, since G contains at most one sprout more than G' , it follows that $d_{\text{AD}}(N, N') \leq d_{\text{AD}}(N, N'') + 1 \leq d$. The case where N' is obtained from N'' by pruning an h-sprout works analogously.

Second, assume that N' has been obtained from N'' by a PR^- that removed the edge $e = (u, v)$. Note that then G' contains $l + 1$ disagreement edges. Assume G' contains a disagreement edge $E_j = (\bar{x}, \bar{y})$ that maps to a path P that contains e in the agreement embedding of G' into N'' . Note that u is a tree vertex and v a reticulation. Therefore, if P contains u as internal vertex, then a t-sprout \bar{w} is attached to E_j in N'' and is mapped to u . Apply an embedding change with regards to \bar{w} and \bar{x} . Handle the case where P contains v as internal vertex analogously. Then E_j is mapped precisely to e . Hence, obtain G from G' by removing E_j . The agreement embedding of G into N is then the same as of G' and the agreement embedding of G into N' is derived from that of G' into N'' by removing E_j . Now assume that e is not covered by a disagreement edge of G' . Let $\bar{e} = (\bar{x}, \bar{y})$ be the edge of G' that covers e . With Lemma 3.3 prune \bar{e} at \bar{x} and \bar{y} such that the resulting graph G'' has at most two sprouts more than G' and an agreement embedding into both N and N'' . Consider \bar{e} now a disagreement edge of G'' and consider a disagreement edge of G'' an agreement subgraph. Then apply the previous case to obtain G . In either case, G contains one disagreement edge less and at most two sprouts more in its agreement subgraphs and therefore $d_{\text{AD}}(N, N') \leq d_{\text{AD}}(N, N'') + 2 - 1 \leq d$.

Lastly, assume N' has been obtained from N'' by a PR^+ . If $l > 0$, obtain G from G' by adding one disagreement edge. If $l = 0$, then G' contains one disagreement edge. Thus obtain G from G' by considering this disagreement edge an agreement subgraph. In either case, it is straightforward to find agreement embeddings of G into N and N' . Since G contains either one disagreement edge more or two sprouts more but one disagreement edge less, it follows again that $d_{\text{AD}}(N, N') \leq d$. This completes the proof. \square

Let $N, N' \in \mathcal{N}_n$ with a maximum agreement graph $G = (V_G, E_G)$. Fix agreement embeddings of G into N and N' and assume that they fulfill the properties of Lemma 3.2. In the proof of the upper bound we will construct a PR-sequence based on agreement embeddings of G along this sequence. To ease talking about PR operations on networks along the sequence based on vertices and edges of G we define the following terminology. Let $\bar{u} \in V_G$ be a t-sprout with outgoing edge $\bar{e} = (\bar{u}, \bar{v}) \in E_G$. Let $e = (u, v)$ be the first edge on the path in N to which \bar{e} is mapped. *Pruning* \bar{u} in N then means that the edge e gets pruned at u . *Regrafting* \bar{u} to an edge $\bar{f} \in E_G$ in N then means that e gets regrafted to the edge $\bar{f} \in E_N$ that is the first edge on the path to which \bar{f} is mapped. Let \bar{x} be a indegree two, outdegree zero vertex or the singleton labelled ρ of G . *Regrafting* \bar{u} to a vertex $\bar{x} \in V_G$ in N then means that e gets regrafted

to the edge $f \in E_N$ that is the outgoing edge of the vertex x to which \bar{x} is mapped. The terminology for h-sprouts is analogously defined. More precisely, the differences for an h-sprout \bar{u} are that the edge \bar{e} is the incoming edge of \bar{u} , and that f is the last edge of the respective path to which \bar{f} is mapped or the incoming edge of the tree vertex x .

We say a sprout \bar{u} is *prunable* (with respect to N) if it is attached to an edge \bar{e} in N and *unprunable* if it is attached to a vertex \bar{x} in N . Let \bar{u} be a sprout that is attached to an edge \bar{f} (or vertex \bar{x}) in N' . We say the sprout \bar{u} is *blocked* if regrafting it to \bar{f} (or \bar{x}) in N would create a directed cycle; otherwise we call it *unblocked*. This implies that there is at least one sprout $\bar{v} \in V_G$ on the path from \bar{u} to \bar{f} (or \bar{x}) in the embedding of G into N . We call such a sprout \bar{v} *blocking*. See Figure 12 (a) and (b) for examples.

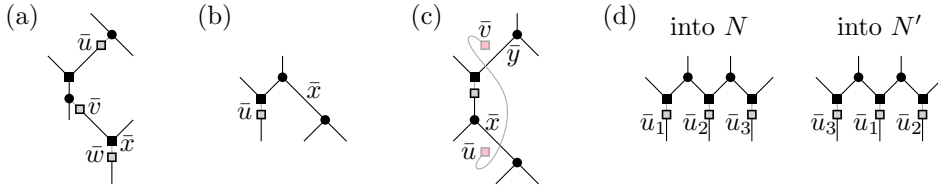


Fig. 12: Embeddings of G into N (and N' in (d)). In (a), the sprout \bar{u} is prunable, but blocked by the blocking sprout \bar{v} if \bar{u} is supposed to take the place of \bar{w} . In (b), \bar{u} is unprunable, but unblocked. In (c), the disagreement edge (\bar{u}, \bar{v}) is not addable since \bar{y} is ancestor of \bar{x} . In (d), the sprouts $\bar{u}_1, \bar{u}_2,$ and \bar{u}_3 form a replacing cycle.

Let $E_i = (\bar{u}, \bar{v})$ be a disagreement edge and \bar{x} and \bar{y} be the vertices or edges to which \bar{u} and \bar{v} , respectively, are attached to in N' . If \bar{x} or \bar{y} is a disagreement edge E_j , then E_i can not be added to N before E_j . Furthermore, if \bar{y} is an ancestor of \bar{x} in the embedding into N , adding E_i to N would create a directed cycle. Therefore we call a disagreement edge $E_i = (\bar{u}, \bar{v})$ *addable* if \bar{y} is not an ancestor of \bar{x} in N and neither \bar{x} nor \bar{y} is a disagreement edge. For example, the edge (\bar{u}, \bar{v}) in Figure 12 (c) is not addable.

If \bar{u} is a sprout attached to a vertex \bar{x} in N , then there is a sprout \bar{v} that is attached to \bar{x} in N' . We say that \bar{v} *takes the place* of \bar{u} . This allows us to define a *replacing sequence* $(\bar{u}_1, \dots, \bar{u}_k)$ of sprouts such that \bar{u}_i takes the place of \bar{u}_{i+1} with regards to N and N' . If furthermore \bar{u}_k takes the place of \bar{u}_1 , then we call it a *replacing cycle*. See Figure 12 (d) for an example. Note that in a replacing sequence the sprout \bar{u}_1 can be the sprout of a disagreement edge.

Theorem 5.3. *Let $N, N' \in \mathcal{N}_n$. Then $d_{\text{PR}}(N, N') \leq 3 d_{\text{AD}}(N, N')$.*

Proof: Let $N, N' \in \mathcal{N}_n$ with r and r' reticulations, respectively. Without loss of generality, assume that $r' \geq r$ and let $l = r' - r$. Let G be a maximum agreement graph for N and N' . Let S_1, \dots, S_k be the agreement subgraphs of G and E_1, \dots, E_l be the disagreement edges of G . Fix agreement embeddings of G into N and into N' . For the embedding into N' , assume that it fulfills the properties of Lemma 3.2. That is, no sprout of an agreement subgraph S_i is attached to a disagreement edge E_j , that at least one disagreement edge (if one exists) is not attached to any other disagreement edge, and that E_i may be attached to E_j only if $j < i$.

Let $d = d_{\text{AD}}(N, N')$. To prove the statement we show how to construct a PR-sequence

$$\sigma = (N = N_0, N_1, \dots, N_m = N')$$

with $m \leq 3d$. While G has an agreement embedding into N and N' , it may not have an agreement embedding for several N_i , $i \in \{1, \dots, m-1\}$. However, starting at $N = N_0$, we preserve the mapping of vertices and edges of G to vertices and paths of N_{i-1} to N_i with each step. Furthermore, along the sequence we map disagreement edges of G to newly added edges. In some cases, it is necessary to add edges to N_{i-1} to obtain N_i with a PR^+ to which no disagreement edge will be mapped. We call such edges *shadow edges*. From each N_{i-1} to an N_i we only prune edges at a vertex in N_i to which a sprout and its incident edge are mapped, or add a disagreement edge, or add or alter a shadow edge. We describe any change of G , or of the embeddings of G into N_i or N' explicitly.

To keep track of the length m of σ , we credit every PR operation either to a sprout or to a disagreement edge. When we obtain $N_m = N'$, each sprout and each disagreement edge will have a credit of at most three and, hence, $m \leq 3d$. Now, assume σ has been constructed up to N_{i-1} .

To obtain N_i we apply the first applicable case of those described below to a sprout or to a disagreement edge. Overall the strategy is to first handle easy cases, that is prunable, unblocked sprouts (Case (A) and (A')) and addable disagreement edges (Case (B) and (B')). Then Case (C), (C') and (C'') handle unprunable, unblocked sprouts. With Case (D) prunable, blocking sprouts are moved "aside" to make them non-blocking and Case (D') adds disagreement edges whose h-sprouts starts a replacing sequence of h-sprouts. After exhaustively applying Case (D) and (D'), we can prove that there always exists a prunable sprout (if any sprouts are left). A particular sprout (resp. disagreement edge) is subject of at most one application of Case (D) (resp. (D')) and one other case.

(A) Prunable, unblocked sprout to non-shadow edge. If there is a prunable, unblocked sprout \bar{u} in N_{i-1} , then obtain N_i by pruning \bar{u} in N_{i-1} and regrafting it to the edge \bar{f} or vertex \bar{x} to which \bar{u} is attached in N' . This step gives \bar{u} a credit of one operation. If \bar{u} is regrafted to a vertex \bar{x} , let \bar{v} be the sprout that is attached to \bar{x} in N_i (i.e., \bar{u} takes the place of \bar{v}). Apply an embedding change of G into N with respect to \bar{u} and \bar{v} . This whole step is illustrated in Figure 13. Note that \bar{u} is now attached either to the same edge \bar{f} or the same vertex \bar{x} in both N_i and N' . Therefore, for the rest of the proof, fix \bar{u} to \bar{f} or identify \bar{u} with \bar{x} , respectively, in G . As a result, \bar{u} with a credit of only one is now not a sprout anymore and thus not subject of another case.

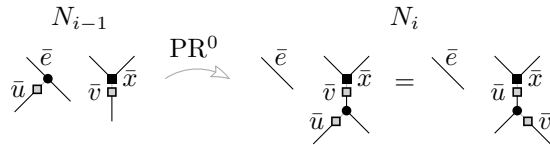


Fig. 13: Illustration of Case (A) where a prunable unblocked sprout \bar{u} gets regrafted to a vertex \bar{x} , and the subsequent embedding change with regards to \bar{u} and \bar{v} .

(B) Addable disagreement edge without shadow edge. If there exists an addable disagreement edge E_j for N_{i-1} , then obtain N_i by adding E_j to N_{i-1} with a PR^+ . This step gives E_j a credit of one operation. If a sprout of E_j is attached to a vertex in N' , then apply again embedding changes of G into N_i like in Case (A). Note that E_j is now attached to the same vertices or edges in both N_i and N' . Therefore, merge the sprouts of E_j with the vertices or edges they are attached to in G . As a result, E_j with a credit of only one is now no disagreement edge anymore, but an edge of an agreement subgraph $S_{j'}$ of G . It will therefore not get any further credit.

(C) Sprout at root, add shadow edge. If there is an unprunable t-sprout \bar{v} attached to the root ρ in

N_{i-1} , then there is another t-sprout \bar{u} that is attached to the root in N' . Assume that \bar{u} is a sprout of a disagreement edge (\bar{u}, \bar{w}) in N' , but that Case (B) does not apply. Then \bar{w} must be attached to another disagreement edge in N' . This however can be changed with embedding changes (like in Lemma 3.2) such that (\bar{u}, \bar{w}) becomes addable and Case (B) applies. Therefore assume \bar{u} is a sprout of an agreement subgraph. Since Case (A) does not apply and the root is an ancestor of \bar{u} , it follows that \bar{u} is an unprunable, but unblocked t-sprout in N_{i-1} . Let \bar{y} be the in-degree two, out-degree zero vertex to which \bar{u} is attached in N_{i-1} . We now obtain N_i from N_{i-1} by adding and attaching a shadow edge (\bar{w}, \bar{z}) from the outgoing edge of \bar{u} to the incoming edge of leaf 1 with a PR^+ . After an embedding change of G into N_i with respect to \bar{w} and \bar{u} , the sprout \bar{u} becomes prunable. Give \bar{u} a credit of one and apply Case (A) to obtain N_{i+1} . In total, \bar{u} gets a credit of two and in N_{i+1} and N' no sprout is attached to the root anymore. This whole step is illustrated in Figure 15. As mentioned above, the embedding of G into N_{i+1} does not cover all edges anymore, since no edge is mapped to the shadow edge.

(C') Sprout at leaf, add shadow edge. This case is analogous to Case (C) but for h-sprouts. Here, if there is an unprunable h-sprout \bar{v} attached to a leaf l in N_{i-1} , then there is another unprunable, unblocked h-sprout \bar{u} that takes the place of \bar{v} . Then obtain N_i again by adding a shadow edge from the outgoing edge of ρ to the incoming edge of \bar{u} . After applying an embedding change, obtain N_{i+1} by pruning \bar{u} and attaching it to the incoming edge \bar{f} of \bar{v} . After another embedding change, merge \bar{u} with the leaf l . If $l = 1$ and there is a shadow edge (\bar{w}, \bar{z}) attached to \bar{f} , then attach \bar{u} above \bar{z} to \bar{f} . This way, \bar{z} is attached to the incoming edge of $l = \bar{u}$ and not to the incoming edge of \bar{v} after the embedding change.

(A') Prunable, unblocked sprout to shadow edge. If after the previous two cases, there is again a prunable, unblocked sprout \bar{u} , apply Case (A) again. However, if in this process \bar{u} gets regrafted to a shadow edge incident to the vertex \bar{x} , then remove the shadow edge with a PR^- after the embedding change of Case (A). This results in a total credit of two for \bar{u} – one for the PR^0 to move \bar{u} and one for the PR^- .

(B') Addable disagreement edge with shadow edge. Similarly, if there is now an addable disagreement edge $E_j = (\bar{u}, \bar{v})$, apply Case (B) in the following way. Assume that \bar{v} of E_j is supposed to get regrafted to a vertex \bar{y} with an incoming shadow edge $\bar{f} = (\bar{w}, \bar{z})$. Then apply a PR^0 to N_{i-1} to prune \bar{f} at \bar{w} and regraft it where \bar{u} is supposed to be attached. Then again, if \bar{u} is supposed to be attached to a vertex \bar{x} with an outgoing shadow edge \bar{f}' , remove \bar{f}' with a PR^- operation after an embedding change. This step is illustrated in Figure 14. The case where only \bar{u} is supposed to be attached to a vertex with an incident shadow edge but not \bar{v} is handled analogously. If there is no shadow edge involved for either \bar{u} or \bar{v} , then Case (B) directly applies. In either case, the total credit for E_j is at most two.

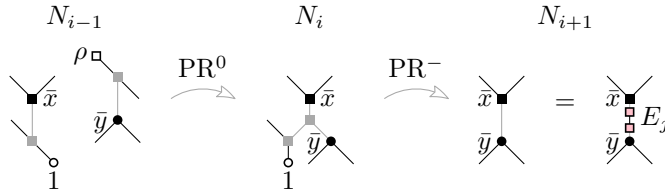


Fig. 14: Illustration of Case (B') with two shadow edges.

The next case is used to decrease the number of blocking sprouts.

(D) Blocked and blocking, but prunable sprout. Let \bar{u} be a prunable, blocked sprout that is blocking

another sprout in N_{i-1} . Then obtain N_i from N_{i-1} by pruning \bar{u} and regrafting it to the outgoing edge of ρ if \bar{u} is a t-sprout, or to the incoming edge of leaf 1 otherwise. Note that \bar{u} is now not blocking any other sprout in N_i . This step gives \bar{u} a credit of one. Later on, \bar{u} will get one or two more credit, depending on whether Case (A) or (A') will apply to it.

(D') Non-addable disagreement edges attached to vertex. Let $E_j = (\bar{u}, \bar{v})$ be a non-addable disagreement edge for which \bar{v} is attached to a vertex \bar{x} in N' . That means that a replacing sequence of h-sprouts starts with \bar{v} of E_j – we change this now. Obtain N_i from N_{i-1} by adding an edge (\bar{u}, \bar{v}) from the outgoing edge of ρ to the incoming edge of \bar{x} . Identify E_j with this new edge and then, after an embedding change, merge \bar{v} with \bar{x} . The vertex \bar{u} is now a non-blocking and prunable, but blocked t-sprout with a credit of one (just like the sprouts of Case (D)). Note that, after Case (D') does not apply anymore, there can be no replacing sequence of h-sprouts that starts with a sprout of a disagreement edge left. (We do not, maybe even cannot, do the analogous for disagreement edges that start a replacing sequence of t-sprouts.)

Applying Case (A) or Case (A') may now start with a sprout that has already a credit of one. However, as in both cases the credit is increased by at most two, the credit will afterwards be at most three.

So far we have applied Case (A) and (B) until not further possible. Then Case (C) and (C') are applied at most once and n times, respectively. We then apply Cases (A), (A'), (B), (B') as long as possible. If then applicable we apply Case (D) or (D') and repeat this loop. Next, we show that if neither of the previous cases applies but there are still sprouts in N_{i-1} that there is then at least one unprunable, unblocked sprout in N_{i-1} .

Existence of unblocked sprout. Assume that there exists a replacing cycle τ of, without loss of generality, t-sprouts in N_{i-1} . Then note that for a t-sprout to be blocked the vertex or edge it will be attached to has to be a descendant. Since phylogenetic networks are acyclic, the sprouts in τ can not all replace a descendant. Therefore one of the sprouts has to be an unblocked sprout.

Next, assume that there is no replacing cycle in N_{i-1} . If no unprunable t-sprout \bar{u} exists, then the h-sprout with no ancestor h-sprout in N_{i-1} is an unblocked sprout. So assume otherwise and let \bar{u} be an unprunable t-sprout with no descendant t-sprout in N_{i-1} . If \bar{u} is unblocked, we are done; so assume otherwise. This means that the vertex or edge to which \bar{u} is supposed to be regrafted is a descendant of \bar{u} in N_{i-1} . Thus, by the choice of \bar{u} , it can only be blocked by an h-sprout \bar{v} . Since Case (D) moved prunable, blocking sprouts aside, \bar{v} has to be unprunable. If \bar{v} is unblocked, we are done; so assume otherwise. Then there is a replacing sequence $\tau = (\bar{v}_1, \dots, \bar{v}_m)$ with $\bar{v} = \bar{v}_i$ for some $i \in \{2, \dots, m\}$. Note that \bar{v}_1 is prunable since Case (D') does not apply and since there are no replacing cycles anymore and thus $\bar{v} \neq \bar{v}_1$. Since further Case (D) does not apply, \bar{v}_1 is also not a blocking sprout. Assuming that there is no unblocked sprout in τ , we know that for every $1 \leq j < i$ the h-sprouts \bar{v}_1 to \bar{v}_j are all descendants of \bar{v}_{j+1} to \bar{v}_i and thus also of \bar{u} . Since \bar{v}_1 is blocked, there has to be an unprunable h-sprout \bar{v}' blocking \bar{v}_1 . Note that \bar{v}' is a descendant of \bar{v}_2 and thus not in τ . The situation with \bar{v}' is now the same as with \bar{v} and the chain of descendants of h-sprouts below \bar{u} contains now $\bar{v} = \bar{v}_i, \dots, \bar{v}_2, \bar{v}'$. Finally, we either find an unprunable h-sprout in the replacing sequence $\tau' \neq \tau$ that contains \bar{v}' or the chain of descendants of h-sprouts below \bar{u} grows longer with h-sprouts \bar{v}'_2 and \bar{v}'' . Since N_{i-1} is finite this chain cannot grow indefinitely and thus at some point we find an unblocked h-sprout.

(C'') Unprunable, unblocked sprout. If there is an unprunable, unblocked sprout \bar{u} in N_{i-1} that is attached to the edge \bar{f} or a vertex \bar{x} in N' that has no shadow edge attached in N_{i-1} , then use the same procedure as in Case (C) or (C') to obtain N_i and then N_{i+1} . This gives \bar{u} a credit of two, before it gets merged with \bar{x} or \bar{f} . This step is illustrated in Figure 15.

If there is an unprunable, unblocked sprout \bar{u} in N_{i-1} that is attached to a vertex \bar{x} in N' that has a

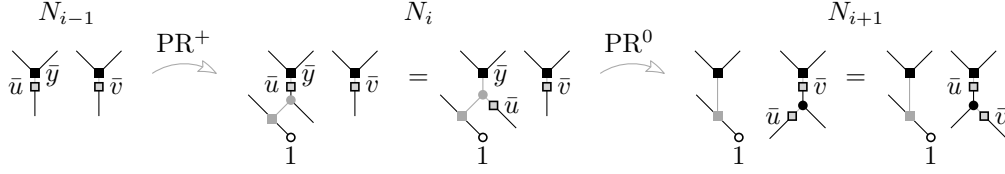


Fig. 15: Illustration of Case (C) and Case (C'') where an unprunable, unblocked sprout \bar{u} is moved to the vertex \bar{x} with two PR operations and two embedding changes.

shadow edge attached in N_{i-1} , then apply the process shown in Figure 16 to obtain N_i and N_{i+1} . This gives \bar{u} a credit of two, before it gets merged with \bar{x} . Note that this moves the shadow edge from \bar{x} to the vertex to which \bar{u} was attached to in N_{i-1} .

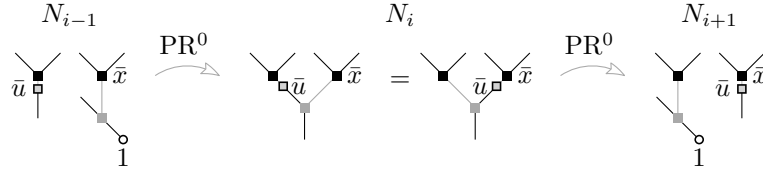


Fig. 16: Illustration of Case (C'') where an unprunable, unblocked sprout \bar{u} is moved to a vertex \bar{x} with an incident shadow edge.

Since prunable sprouts cannot block after they got moved aside, since disagreement edges cannot block either (by the properties of the agreement embedding into N'), and since the number of unprunable sprouts is decreased stepwise, the whole process resolves all sprouts and disagreement edges. Hence, $N_m = N'$. Since every sprout and every disagreement edge got a credit of at most three, it follows that $m \leq 3d$. This concludes the proof. \square

We prove a relation between the PR-distance and the SNPR-distance.

Lemma 5.4. *Let $N, N' \in \mathcal{N}_n$. Then*

$$d_{PR}(N, N') \leq d_{SNPR}(N, N') \leq 2 d_{PR}(N, N').$$

Proof: The first inequality follows from the definitions of PR and SNPR. For the second inequality, let $d = d_{PR}(N, N')$ and $\sigma = (N = N_0, N_1, \dots, N_d = N')$ be a PR-sequence from N to N' of length d . Then we can construct an SNPR-sequence $\sigma^* = (N = M_0, M_1, \dots, M_k = N')$ with $k \leq 2d$ as follows. Assume we have constructed σ^* up to $M_{j-1} = N_{i-1}$. Then, if N_i is obtained from N_{i-1} by a tail PR^0 or a PR^- , then apply the same operation to M_{j-1} to obtain M_j . So assume, otherwise; i.e., N_i is obtained from N_{i-1} by a head PR^0 . Let $e = (u, v)$ be the edge that gets pruned at v and f be the edge that gets subdivided to regraft e . Obtain M_i from M_{j-1} with the $SNPR^+$ that subdivides e with a new vertex u' , subdivides f with a new vertex v' , and adds the edge (u', v') . Next, obtain M_{i+1} from M_i by removing (u', v) and suppressing the resulting degree two vertices. Then clearly $M_{i+1} = N_i$. Since at most two SNPR operations are needed per PR, it follows that $k \leq 2d$. \square

The following corollary is a direct consequence of Theorems 5.2 and 5.3 and Lemma 5.4.

Corollary 5.5. *Let $N, N' \in \mathcal{N}_n$. Then*

$$d_{\text{AD}}(N, N') \leq d_{\text{SNPR}}(N, N') \leq 6 d_{\text{AD}}(N, N').$$

6 Concluding remarks

In this paper, we defined maximum agreement graphs for two rooted binary phylogenetic networks. Like maximum agreement forests for trees, a maximum agreement graph models how the two networks agree on subgraphs derived from a minimum number of prunings. If the two networks have different numbers of reticulations, then agreement graphs also model how they disagree on that. Based on this, we defined the agreement distance on phylogenetic networks. First, we showed that the agreement distance equals the rSPR-distance when calculated for phylogenetic trees. For phylogenetic networks, the agreement distance is a lower bound on the PR- and SNPR-distance. Furthermore, it bounds both the PR- and SNPR-distance from above by a factor of at most three and six, respectively. These upper bounds might not be tight. For example, for the PR-distance the bound might be closer to twice the agreement distance. This thought is also motivated by the fact that the neighbourhoods of a network under PR and the agreement distance are the same.

While the agreement distance is still NP-hard to compute, it avoids problems of shortest PR- or SNPR-sequences as identified by Klawitter and Linz (2019). While for such a shortest sequence it might matter at which step of the sequence a reticulation edge is added, an agreement graph has simply as many disagreement edges as needed. Furthermore, while a sequence might traverse networks with more or less reticulations than the start and target network, this is also irrelevant for agreement graphs. Moreover, the SNPR-distance between two networks of a certain class, for example of tree-child networks, can differ if considered in the space of \mathcal{N}_n or just within this class, i.e., where the SNPR-sequence does not leave the class. This is by definition not the case for the agreement distance. We therefore hope that it is easier to find exact and approximation algorithms for the agreement distance than for the PR-distance, just as it has been more fruitful to work with agreement forests than with shortest rSPR-sequences.

Beyond rooted binary phylogenetic networks it is interesting to see whether agreement graphs and the agreement distance can be generalised to multifurcating phylogenetic networks or even to directed graphs in general. For unrooted phylogenetic trees, Allen and Steel (2001) have shown that unrooted agreement forests characterise the distance of the tree bisection and reconnection (TBR) operation. This imposes the questions whether agreement graphs can also be defined for unrooted phylogenetic networks and how they would relate to generalisations of the (unrooted) SPR and the TBR operation.

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