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# On the complexity of optimising variants of phylogenetic diversity on phylogenetic networks

Magnus Bordewich<sup>a,\*</sup>, Charles Semple<sup>b</sup>, Kristina Wicke<sup>c</sup>

<sup>a</sup> Department of Computer Science, Durham University, United Kingdom

<sup>b</sup> School of Mathematics and Statistics, University of Canterbury, Christchurch, New Zealand

<sup>c</sup> Department of Mathematics, The Ohio State University, Columbus, OH, USA

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# ABSTRACT

Phylogenetic Diversity (PD) is a prominent quantitative measure of the biodiversity of a collection of present-day species (taxa). This measure is based on the evolutionary distance among the species in the collection. Loosely speaking, if  $\mathcal{T}$  is a rooted phylogenetic tree whose leaf set X represents a set of species and whose edges have real-valued lengths (weights), then the PD score of a subset S of X is the sum of the weights of the edges of the minimal subtree of  $\mathcal T$  connecting the species in S. In this paper, we define several natural variants of the PD score for a subset of taxa which are related by a known rooted phylogenetic network. Under these variants, we explore, for a positive integer k, the computational complexity of determining the maximum PD score over all subsets of taxa of size k when the input is restricted to different classes of rooted phylogenetic networks.  $^{\odot}$  2022 The Authors. Published by Elsevier B.V. This is an open access article under the

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# 1. Introduction

Phylogenetic diversity (PD) is a popular measure for quantifying the biodiversity of a set of species based on their evolutionary history and relatedness. Roughly speaking, the PD score of a group of species (taxa) quantifies how much of the 'tree of life' is spanned by the species in the group. Ever since its introduction by Daniel Faith in 1992 [8], this metric has attracted great attention in the literature both among empiricists and theorists. Indeed, Faith's seminal paper has been cited in excess of 2000 times.

In the face of limited resources in biodiversity conservation, a central problem in relation to phylogenetic diversity is to identify subsets of species that maximise the PD score. While there are efficient algorithms for finding maximum PD sets on a given tree [15,20,27], variants of the problem (e.g., maximising PD across several trees [3,26] or incorporating conservation costs and extinction probabilities in the so-called 'Noah's ark problem' [28]) have led to many interesting algorithmic questions. Most of this work to date has focused on measuring and maximising PD on phylogenetic trees. However, the metric has been extended to and analysed for so-called split networks [2,7,16,17,26] which are typically used to represent conflicts in data. More recently, the authors in [29] have suggested approaches to measuring PD on explicit phylogenetic networks, which represent the evolutionary histories of collections of species whose past include reticulation (non-treelike) events such as hybridisation and horizontal gene transfer.

As processes such as hybridisation pose new challenges to biodiversity conservation (e.g., [19,21]) and diversity measures beyond PD on phylogenetic trees are needed, in this paper we present the first rigorous analysis of the computational

E-mail addresses: m.j.r.bordewich@durham.ac.uk (M. Bordewich), charles.semple@canterbury.ac.nz (C. Semple), wicke.6@osu.edu (K. Wicke).

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\* Corresponding author.

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complexity of optimising variants of phylogenetic diversity extended to rooted phylogenetic networks. These results could lead to algorithms that aid conservationists and policy makers in making more accurately informed decisions. We extend the work of [29] and define four natural variants of the PD score for a subset of taxa whose evolution is described by a rooted phylogenetic network  $\mathcal{N}$ . We explore the relationships between these four measures and then analyse the computational complexity of, given  $\mathcal{N}$  and a positive integer k, determining the maximum PD score over all subsets of taxa of size k under these variants of PD and for different classes of rooted phylogenetic networks.

The main results of this paper are as follows. We show that the complexity of determining the maximum AllPaths-PD score, our first variant of PD for rooted phylogenetic networks, depends on the class of networks to which  $\mathcal{N}$  belongs. In particular, for tree-child networks the optimisation problem is hard, whereas for level-1 networks the problem is polynomial (see Section 4). In Section 5 we introduce a second variant, Network-PD, which, in contrast to AllPaths-PD, takes into account the proportion of features a reticulation vertex inherits from each of its parents. We show that Network-PD is a generalisation of AllPaths-PD, and thus the corresponding optimisation problem is again computationally hard in general. In addition, we show that there is a direct correspondence between the maximum and minimum of Network-PD, and the third and fourth variants of PD for phylogenetic networks considered in this manuscript, namely MaxWeightTree-PD and MinWeightTree-PD. We end the paper by analysing the latter two more in-depth. More precisely, we show that the problem of determining the maximum value over all subsets of taxa of size *k* is solvable in polynomial time for MaxWeightTree-PD even computing the MinWeightTree-PD score of a fixed subset of *X* is computationally hard, and hence the optimisation problem is also hard (Section 7).

Before the main results, in Section 2 we give formal definitions of the structures and notation used throughout this manuscript. After reviewing the concept of PD on rooted phylogenetic trees, we then formally introduce our four variants of PD on rooted phylogenetic networks in Section 3. As described above, the remaining sections are devoted to analysing the complexity of determining the maximum PD score over all subsets of taxa of size k under these four variants of PD and when the input is restricted to different classes of rooted phylogenetic networks.

## 2. Notation and preliminaries

To formally state our results, we need some notation and terminology. Throughout the paper, X denotes a non-empty finite set (of taxa).

*Phylogenetic networks* A rooted binary phylogenetic network N on X is a rooted directed acyclic graph with no parallel arcs satisfying the following properties:

- (i) the (unique) root has in-degree zero and out-degree two;
- (ii) a vertex with out-degree zero has in-degree one, and the set of vertices with out-degree zero is X; and
- (iii) all other vertices have either in-degree one and out-degree two, or in-degree two and out-degree one.

For technical reasons, if |X| = 1, we allow  $\mathcal{N}$  to consist of the single vertex in X. The vertices in X are *leaves*. We call X the *leaf set* of  $\mathcal{N}$  and frequently denote it by  $\mathcal{L}(\mathcal{N})$ . The vertices with in-degree one and out-degree two are *tree vertices*, while the vertices with in-degree two and out-degree one are *reticulations*. We refer to arcs directed into a reticulation as *reticulation arcs* and to all other arcs as *tree arcs*. Furthermore, throughout the paper, we assume that all arcs of  $\mathcal{N}$  have non-negative real-valued lengths, that is, if A denotes the arc set of  $\mathcal{N}$ , then associated with  $\mathcal{N}$  is a mapping  $w : A \to \mathbb{R}^{\geq 0}$  under which each arc e of  $\mathcal{N}$  is assigned the weight w(e). As, for instance, indicated by [10], the underlying meaning of these arc lengths is often context-dependent, and ranges from the expected number of substitutions per site, to coalescent units, to the amount of (calendar) time elapsed. To illustrate, three rooted binary phylogenetic networks are shown in Fig. 1. Here, as in all figures in the paper, arcs are directed down the page. A *rooted binary phylogenetic X-tree* is a rooted binary phylogenetic network on X with no reticulations. For the remainder of the paper, we will refer to rooted binary phylogenetic trees, respectively, as all such networks and trees considered are rooted and binary.

We remark here that we have presented the arguments in this paper in terms of binary phylogenetic networks, both for simplicity of understanding and because the hardness results are stronger. However, we note that the results extend to phylogenetic networks whose non-leaf vertices have either in-degree one and out-degree at least two, or in-degree two and out-degree one. This is discussed further in Section 8.

*Tree-child and level-1 networks* A phylogenetic network  $\mathcal{N}$  on X is a *tree-child network* [6] if each non-leaf vertex is the parent of a tree vertex or a leaf. Equivalently,  $\mathcal{N}$  is tree-child if (i) no tree vertex is the parent of two reticulations and (ii) no reticulation is the parent of another reticulation [25]. And again, equivalently,  $\mathcal{N}$  is tree-child if, for every vertex v of  $\mathcal{N}$ , there is a path from v to a leaf  $\ell$  that consists only of tree vertices (except  $\ell$  and possibly v itself). We call such a path a *tree path.* 

Let  $\mathcal{N}$  be a phylogenetic network. A reticulation arc (u, v) of  $\mathcal{N}$  is called a *shortcut* if there is a directed path in  $\mathcal{N}$  from u to v that avoids (u, v). We say that  $\mathcal{N}$  is a *normal network* [30] if it is tree-child and has no shortcuts. Finally,  $\mathcal{N}$  is a



**Fig. 1.** Phylogenetic tree  $\mathcal{T}$  and tree-child networks  $\mathcal{N}$  and  $\mathcal{N}'$  on  $X = \{x_1, \dots, x_6\}$  with non-negative real-valued arc weights. Note that  $\mathcal{N}$  is normal but not level-1, whereas  $\mathcal{N}'$  is level-1 but not normal (due to the shortcut (u, v)).

*level-1 network* if its underlying (undirected) cycles are vertex disjoint. Normal and level-1 networks are proper subclasses of tree-child networks. An example of two tree-child networks, one normal and the other level-1, is shown in Fig. 1.

*Connecting subtrees* Let  $\mathcal{N}$  be a phylogenetic network on X with root  $\rho$ , and let  $Y \subseteq X$ . We call any subgraph T of  $\mathcal{N}$  that is a directed rooted tree (i.e. an arborescence) with root  $\rho$  and leaf set Y, a *connecting subtree for* Y. Note that  $\rho$  may have out-degree one in T. Moreover, there might be several connecting subtrees for Y in  $\mathcal{N}$ . We denote the set of all connecting subtrees for Y in  $\mathcal{N}$  as  $T_Y(\mathcal{N})$ . Also note that any connecting subtree T for Y is an edge-weighted tree, where each edge  $e \in T$  inherits its weight w(e) from  $\mathcal{N}$ .

# 3. Variants of phylogenetic diversity for phylogenetic networks

In this section, we introduce our variants of PD for phylogenetic networks and then consider the associated optimisation problems.

# 3.1. PD on phylogenetic trees and phylogenetic networks

Before we define variants of PD for phylogenetic networks, we briefly review PD for phylogenetic trees. Phylogenetic diversity arose as a quantitative measure of the biodiversity of a set of species for use in conservation decisions [8]. PD has been studied for a variety for organisms, ranging from bacteria [13], to plants [4], to mammals [24]. Moreover, the *International Union for Conservation of Nature* (IUCN) has established a 'Phylogenetic Diversity Task Force' aiming at promoting the use of PD in conservation decisions (see https://www.pdtf.org/). PD also serves as a basis for so-called phylogenetic diversity indices such as the 'Fair Proportion index' [22] (also called 'evolutionary distinctiveness score' [11]) and the 'Equal Splits index' [22,23] that rank species for conservation, based on their contribution to overall PD. These indices are used in conservation initiatives such as the 'EDGE of Existence programme' established by the Zoological Society of London [11].

The key underlying assumption in the use of PD as a quantitative measure is that if the arcs of a phylogenetic tree are weighted according to genetic distance, then features of interest (be that biological, pharmaceutical or conservational) will have arisen at a rate proportional to the lengths of the arcs. A further assumption is that all features that arose in an ancestral species have persisted to be present in the extant species descended from them. So the PD score is proportional to the number of distinct features present in a set of species. In particular, let  $\mathcal{T}$  be a phylogenetic *X*-tree (with non-negative real-valued arc lengths). The *phylogenetic diversity* (PD score) of a subset  $S \subseteq X$ , denoted as  $PD_{\mathcal{T}}(S)$ , is the sum of arc lengths in the (unique) connecting subtree for *S* in  $\mathcal{T}$ . Referring to Fig. 1(i), if  $S = \{x_2, x_4, x_6\}$ , then  $PD_{\mathcal{T}}(S) = 15$ .

*AllPaths-PD* There are different ways that the definition of PD may be extended from phylogenetic trees to phylogenetic networks, which we discuss now. The most straightforward approach is to again assume that all features that arise in any ancestral species persist to be present in all descendant extant species; then the natural extension of the PD score to networks is what we have called *AllPaths-PD*. Specifically, for a phylogenetic network  $\mathcal{N}$  and a subset  $S \subseteq X$ , we define

$$AllPaths-PD_{\mathcal{N}}(S) = \sum_{e \in Anc(S)} w(e),$$

where Anc(S) is the set of all arcs that are ancestral to at least one taxon in *S*, i.e. lie on a directed path from the root of N to some leaf in *S*.

*Network-PD* To obtain a more accurate evaluation of the relative feature diversity of different subsets of taxa, we require knowledge of the proportion of features present in a parent species that are inherited by a child species. At a reticulation representing a true hybridisation event, the child taxon might inherit 50% of the features of one parent and 50% of the

features of the other. Whereas, at a reticulation representing a lateral gene transfer, the child may inherit the entire genome of one parent species, i.e. 100% of the features, and also receive an injection of a small section of DNA from the other parent, perhaps 5% of the features. Thus, at each reticulation of our phylogenetic network, we must be given weights on each incoming arc corresponding to the proportion of features of the parent inherited by the child. Given this information, a more accurate measure, which we have called *Network-PD*, may be obtained.

On each incoming arc e = (u, v) to each reticulation v of a phylogenetic network  $\mathcal{N}$ , let p(e) be the *inheritance proportion* (*function*), giving the proportion of features of the parent vertex u that are present in the child vertex v of that arc. We assume that for all reticulation arcs  $p(e) \in [0, 1]$ . (Just as genetic distance is used in the arc lengths of a phylogenetic tree when computing PD as a proxy for the number of features of interest, we could use the proportion of the parental genome present in the child taxon as an estimate for the proportion of parental features inherited by the child.) For a subset S of the leaves of  $\mathcal{N}$ , we define, for each arc  $e = (u, v) \in \mathcal{N}$ , the function  $\gamma(S, e)$  to be the proportion of the features of v that are present in the taxa set S. (Equivalently,  $\gamma(S, e)$  is the probability that a feature arising on arc e is inherited by some taxon in set S). We now define Network-PD as follows:

Network-PD<sub>$$\mathcal{N}, p$$</sub>(S) =  $\sum_{e \in \mathcal{N}} \gamma(S, e) \cdot w(e)$ .

Where the phylogenetic network N or inheritance proportion function p is obvious, we may omit them from the subscript. We may compute  $\gamma(S, e)$  in a bottom up fashion as follows. For e = (u, v),

- (i) if v is a leaf and  $v \in S$  then  $\gamma(S, e) = 1$ , whereas if  $v \notin S$  then  $\gamma(S, e) = 0$ ;
- (ii) if v is a tree vertex with outgoing arcs  $f_1$  and  $f_2$ , then

$$\gamma(S, e) = \gamma(S, f_1) + \gamma(S, f_2) - \gamma(S, f_1)\gamma(S, f_2);$$

(iii) if *v* is a reticulation vertex with outgoing arc *f*, then  $\gamma(S, e) = \gamma(S, f)p(e)$ .

*MaxWeightTree-PD and MinWeightTree-PD* It is likely that, in practice, complete knowledge of the inheritance proportion function p will not be possible, so we may be interested in upper and lower bounds on Network-PD under varying p. Note that if p is allowed to vary without restriction it can still be no more than 1 on each arc, and that setting p = 1 on all arcs gives AllPaths-PD. The inheritance proportion p can also be no less than 0 on any arc, and setting p = 0 on all arcs reduces Network-PD<sub>N</sub> to PD on a phylogenetic tree (specifically PD<sub>T</sub>, where T is, up to isomorphism, the phylogenetic tree obtained by deleting each reticulation arc of N and connecting the reticulation vertices to the root by arcs of weight 0). These extremities of p on Network-PD are thus not (mathematically) interesting in their own right.

However, total inheritance proportions of 0 or 2 at a reticulation are unrealistic. Alternatively, we might assume that each feature inherited from the second parent replaces some feature from the first parent. That is to say, at a reticulation with incoming arcs  $e_1$  and  $e_2$  we require  $p(e_1) + p(e_2) = 1$ . Under this assumption upper and lower bounds for the total quantity of features present in a given subset of taxa are the PD scores of the maximum-weight and minimum-weight connecting subtrees for those taxa. Specifically, for a subset  $S \subseteq X$ , we define the following two variants of PD:

MaxWeightTree-PD<sub>$$\mathcal{N}$$</sub>(S) =  $\max_{T \in \mathsf{T}_{S}(\mathcal{N})} \sum_{e \in T} w(e)$ 

and

MinWeightTree-PD<sub>N</sub>(S) = 
$$\min_{T \in \mathsf{T}_{S}(\mathcal{N})} \sum_{e \in T} w(e).$$

We elaborate further how Network-PD is bounded by MinWeightTree-PD and MaxWeightTree-PD in Section 5.1.

Note that AllPaths-PD is called 'phylogenetic subnet diversity' in [29], MinWeightTree-PD is called 'phylogenetic net diversity', and MaxWeightTree-PD is related to the notion of 'embedded phylogenetic diversity' discussed therein. However, while the authors of [29] introduced and compared different variants of PD for phylogenetic networks, they did not analyse the complexity of, given a phylogenetic network  $\mathcal{N}$  and a positive integer k, computing the maximum PD score over all subsets of taxa of size k, or finding a subset  $S \subseteq X$  of cardinality k which maximises the PD score under these variants. In the following, we consider the first problem, i.e. computing the maximum PD score over all subsets of taxa of size k under the phylogenetic diversity variants introduced above on phylogenetic networks.

#### 3.2. Optimisation problems

The problem of finding a subset of taxa of cardinality k maximising the PD score has been extensively studied on phylogenetic trees. It corresponds to the task in conservation biology of determining which k species maximise the biodiversity of the group [8]. Here, we focus on the problem of computing the maximum PD score over all subsets of taxa of size kunder the variants of PD defined above. More precisely, we study the following optimisation problems:

# **MAX-ALLPATHS-PD**( $\mathcal{N}, k$ ):

**Input:** A phylogenetic network  $\mathcal{N}$  on taxa set X and a positive integer k. **Objective:** Determine the maximum value of AllPaths-PD<sub> $\mathcal{N}$ </sub>(S) over all subsets  $S \subseteq X$  of cardinality k.

# **MAX-NETWORK-PD** $(\mathcal{N}, p, k)$ :

**Input:** A phylogenetic network N on taxa set X, a inheritance proportion function p on the reticulation arcs of N, and a positive integer k.

**Objective:** Determine the maximum value of Network-PD<sub>N, p</sub>(*S*) over all subsets  $S \subseteq X$  of cardinality *k*.

# **MAX-MAXWEIGHTTREE-PD** $(\mathcal{N}, k)$ :

**Input:** A phylogenetic network  $\mathcal{N}$  on taxa set X and a positive integer k. **Objective:** Determine the maximum value of MaxWeightTree-PD<sub> $\mathcal{N}$ </sub>(S) over all subsets  $S \subseteq X$  of cardinality k.

### **MAX-MINWEIGHTTREE-PD**( $\mathcal{N}, k$ ):

**Input:** A phylogenetic network  $\mathcal{N}$  on taxa set X and a positive integer k. **Objective:** Determine the maximum value of MinWeightTree-PD<sub> $\mathcal{N}$ </sub>(S) over all subsets  $S \subseteq X$  of cardinality k.

The complexity of these optimisation problems will be discussed in the sections that follow.

# 4. AllPaths-PD

We begin by studying AllPaths-PD. Let  $\mathcal{N}$  be a phylogenetic network on X. Recall that, for any subset  $S \subseteq X$ , we defined AllPaths-PD $_{\mathcal{N}}(S)$  to be the sum of the weights of all arcs of  $\mathcal{N}$  which lie on a path from the root of  $\mathcal{N}$  to a leaf in S, and MAX-ALLPATHS-PD to be the problem of finding the maximum value of AllPaths-PD $_{\mathcal{N}}(S)$  over all subsets  $S \subseteq X$  of cardinality k.

In this section we show first that, in general, the problem Max-ALLPATHS-PD is NP-hard even when restricted to the class of normal networks. Moreover, we observe that Max-ALLPATHS-PD cannot be approximated within  $1 - \frac{1}{e} \approx 0.632$  unless P = NP, and that a greedy algorithm will achieve this approximation ratio. Second, we show that Max-ALLPATHS-PD can be solved in polynomial time on level-1 networks.

### 4.1. Maximising AllPaths-PD is NP-hard

In order to show that Maximising AllPaths-PD is NP-hard we will use a reduction to the well-known Maximum Coverage problem:

# **MAXIMUM COVERAGE**(S, k):

**Input:** A collection  $S = \{S_1, S_2, ..., S_n\}$  of sets and a positive integer *k*. **Objective:** Find a subset  $S' \subseteq S$  such that |S'| = k and the number of covered elements,  $|\bigcup_{S_i \in S'} S_i|$ , is maximised.

MAXIMUM COVERAGE is NP-hard to solve exactly. Indeed, the inapproximability of MAXIMUM COVERAGE is well studied, and it is known that the approximation threshold is  $1 - \frac{1}{e}$ . That is, unless P = NP, no polynomial-time algorithm exists that always returns a solution to MAXIMUM COVERAGE that is guaranteed to have value greater than  $1 - \frac{1}{e}$  of the optimal solution [9].

**Theorem 4.1.** The problem MAX-ALLPATHS-PD is NP-hard. Moreover, MAX-ALLPATHS-PD cannot be approximated in polynomial time with approximation ratio better than  $1 - \frac{1}{e}$  unless P = NP.

**Proof.** Let S, a collection of sets, and k, a positive integer, be an instance of MAXIMUM COVERAGE. We begin by constructing a phylogenetic network  $\mathcal{N}$  with leaf set S as follows. Set  $E = \bigcup_{S \in S} S$ , that is, E is the ground set of the MAXIMUM COVERAGE instance. Take any phylogenetic tree (a caterpillar would do) with leaf set E, where each internal arc has weight 0 and each pendant arc (i.e. an arc incident with a leaf) has weight 1. The arcs of weight 1 are thus in one-to-one correspondence with the elements in E. Label each of these arcs with the same element of E as its incident leaf. Now, for each  $S \in S$ , (i) add two new vertices S and  $\hat{S}$  to this construction and a new arc ( $\hat{S}$ , S), and (ii), for each  $e \in S$ , add a new arc (e,  $\hat{S}$ ).

This will result in each vertex labelled e, where  $e \in E$ , having out-degree corresponding to the number of sets containing e, and each vertex  $\hat{S}$  having in-degree corresponding to the number of members of S. Next, refine every vertex that has either out-degree at least three or in-degree at least three, so that every resulting vertex has out-degree equal to two or in-degree equal to two, respectively. These new arcs below the arcs of E are all assigned weight 0. Finally, suppress any vertices of in-degree one and out-degree one resulting from an element  $e \in E$  that is only contained in a single member of S, and keep weight 1 and the label e on the newly merged arc. The resulting phylogenetic network on S is N and the construction takes time polynomial in the size of S. See Fig. 2 for an example of the construction.



**Fig. 2.** The network  $\mathcal{N}$  resulting from reducing a MAXIMUM COVERAGE instance  $(\mathcal{S}, k)$  to a MAX-ALLPATHS-PD instance  $(\mathcal{N}, k)$ . In this case,  $\mathcal{S} = \{S_1, S_2, S_3, S_4\}$ , where  $S_1 = \{e_1, e_3, e_4\}, S_2 = \{e_2, e_5, e_6\}, S_3 = \{e_4, e_5, e_7\}$  and  $S_4 = \{e_7, e_8, e_9\}$ , and so  $E = \{e_1, e_2, \dots, e_9\}$ . On the left the network  $\mathcal{N}'$  illustrates the construction before the final step of suppressing the vertices of in-degree one and out-degree one.

Consider a subset S' of the leaves of N. An arc  $e \in E$  is on a path from the root of N to a member S of S' if and only if the set S contains the corresponding element e. Thus the number of arcs in E that lie on paths from the root to a member of S is precisely  $|\bigcup_{S \in S'} S|$ . Since all the arcs of N have weight 0 except those labelled with an element of E which have weight 1,

AllPaths-PD<sub>$$\mathcal{N}$$</sub> $(\mathcal{S}') = \left| \bigcup_{S \in \mathcal{S}'} S \right|.$ 

Thus solving MAX-ALLPATHS-PD is at least as hard as solving MAXIMUM COVERAGE, which is well known to be NP-hard [9].

It is known that the approximation threshold of MAXIMUM COVERAGE is  $1 - \frac{1}{e}$ . Since we have equality in the optimal solutions to the two problems, if a polynomial-time algorithm that approximated MAX-ALLPATHS-PD to a better ratio than  $1 - \frac{1}{e}$  existed, then using the reduction above we would be able to obtain a polynomial-time approximation for MAXIMUM COVERAGE with the same ratio. Thus, unless P = NP, this is not possible. This completes the proof of the theorem.  $\Box$ 

The hardness result of Theorem 4.1 can be extended to show that MAX-ALLPATHS-PD remains NP-hard even when the input phylogenetic network is restricted to be from the class of normal networks.

**Theorem 4.2.** The problem MAX-ALLPATHS-PD is NP-hard even when the inputted phylogenetic network is restricted to be from the class of normal networks.

**Proof.** The construction is the same as used in the proof of Theorem 4.1 with the following additions. Starting from the constructed phylogenetic network N with leaf set S, we transform it into a normal network N' by

- (i) assigning weight 1 to the pendant arcs leading to the leaves of N labelled by elements of S (which we call *original* leaves); and
- (ii) subdividing all reticulation arcs of N with a new vertex and adjoining a new leaf via a new pendant arc with weight 0 to each new vertex (which we call a *new leaf*).

Note that the construction in (ii) means that  $\mathcal{N}'$  is normal [30]. Furthermore, this construction takes time polynomial in the size of  $\mathcal{N}$ . Now observe that, for any subset  $\mathcal{S}'$  of the leaf set of the augmented phylogenetic network  $\mathcal{N}'$ , if  $\mathcal{S}'$  contains a new leaf  $\ell$ , then we may find an original leaf  $\ell'$  that is a descendent of  $\ell$ 's parent vertex. The set  $(\mathcal{S}' \cup \{\ell'\}) - \{\ell\}$  will have an AllPaths-PD score at least as high as that for the set  $\mathcal{S}'$ , since all arcs with weight 1 on a path from the root of  $\mathcal{N}'$  to  $\ell'$ . Moreover, if a subset  $\mathcal{S}'' \subseteq \mathcal{S}$  contains k original leaves, then its AllPaths-PD score is precisely

$$k+\left|\bigcup_{s\in\mathcal{S}''}S\right|.$$

Thus optimal solutions to MAX-ALLPATHS-PD still correspond to optimal subsets of S, and thus MAX-ALLPATHS-PD remains NP-hard even in this restricted case.  $\Box$ 

We next show that AllPaths-PD is a submodular function. From this it will follow that a greedy algorithm yields a guaranteed approximation for MAX-ALLPATHS-PD.

**Lemma 4.3.** Let N be a phylogenetic network on X. Then the function AllPaths-PD, which assigns each subset  $S \subseteq X$  a non-negative real value, is a submodular function, i.e. for all  $A, B \subseteq X$ , we have

AllPaths-PD<sub> $\mathcal{N}$ </sub> $(A \cup B)$  + AllPaths-PD<sub> $\mathcal{N}$ </sub> $(A \cap B) \leq$  AllPaths-PD<sub> $\mathcal{N}$ </sub>(A) + AllPaths-PD<sub> $\mathcal{N}$ </sub>(B).

**Proof.** Recall that, for all  $S \subseteq X$ , Anc(S) is the set of arcs that are ancestral to at least one taxon in S. Thus

AllPaths-PD(S) = 
$$\sum_{e \in \mathcal{N}} \delta(S, e) \cdot w(e),$$

where

$$\delta(S, e) = \begin{cases} 1, & \text{if } e \in \operatorname{Anc}(S); \\ 0, & \text{otherwise.} \end{cases}$$

If  $e \in Anc(A \cup B)$ , then e is on a path from the root of  $\mathcal{N}$  to a leaf in  $A \cup B$ , that is, e is on a path from the root of  $\mathcal{N}$  to a leaf in either A or B. Thus

 $Anc(A \cup B) = Anc(A) \cup Anc(B)$ 

and, similarly,

 $\operatorname{Anc}(A \cap B) \subseteq \operatorname{Anc}(A) \cap \operatorname{Anc}(B).$ 

It follows that, for all arcs e in  $\mathcal{N}$  and all  $A, B \subseteq X$ ,

$$\delta(A \cup B, e) + \delta(A \cap B, e) - \delta(A, e) - \delta(B, e) \le 0.$$

Since

AllPaths-PD $(A \cup B)$  + AllPaths-PD $(A \cap B)$  - AllPaths-PD(A) - AllPaths-PD(B)

is a weighted sum of the corresponding  $\delta$  quantities above with non-negative weights, the statement now follows.  $\Box$ 

Consider the following greedy algorithm for MAX-ALLPATHS-PD. Given a phylogenetic network N on X and an integer k, first select a taxon at maximum distance from the root of N and then iteratively select a taxon that maximises the incremental increase in AllPaths-PD until a total of k taxa have been selected.

**Corollary 4.4.** The greedy algorithm above returns a  $(1 - \frac{1}{e})$  approximation for the MAX-ALLPATHS-PD problem.

**Proof.** By Lemma 4.3, AllPaths-PD is a submodular function. It is also non-decreasing (adding a taxon will never decrease the AllPaths-PD score). Hence it fits the framework of standard approaches to constructing greedy algorithms for cardinality constrained submodular functions studied in [18]. In particular, by [18], it yields an approximation algorithm with approximation ratio  $1 - \frac{1}{e}$ .

Note that, by Theorem 4.1, the approximation ratio in the statement of Corollary 4.4 cannot be improved unless  $P \neq NP$ .

# 4.2. Maximising AllPaths-PD on level-1 networks

Although MAX-ALLPATHS-PD is NP-hard in general, in this section we show that it is polynomial time for the class of level-1 networks. Let  $\mathcal{N}$  be a level-1 network on X. We begin by determining two connecting subtrees  $T_1$  and  $T_2$  for X in  $\mathcal{N}$  that together cover all arcs of  $\mathcal{N}$ . Let v be a reticulation of  $\mathcal{N}$ . Since  $\mathcal{N}$  is level-1, it is easily seen that there is a unique tree vertex, s say, of  $\mathcal{N}$  such that there exist distinct (directed) paths P and P' starting at s and ending at v such that s and v are the only vertices of P and P' in common. We refer to s as the source vertex of v. Now, let  $v_1, v_2, \ldots, v_k$  denote the reticulations of  $\mathcal{N}$ . For each  $i \in \{1, 2, \ldots, k\}$ , let  $s_i$  denote the source vertex of  $v_i$ . Furthermore, for each  $i \in \{1, 2, \ldots, k\}$ , let  $u_i$  and  $u'_i$  denote the (distinct) parents of  $v_i$ . Note that at most one of  $u_i$  and  $u'_i$  is  $s_i$ . Let  $T_1$  be the connecting subtree for X in  $\mathcal{N}$  obtained from  $\mathcal{N}$  by deleting  $(u'_i, v_i)$  for all i, and re-weighting each of the arcs on the (unique) path from  $s_i$  to



**Fig. 3.** (i) A level-1 network  $\mathcal{N}$  on  $X = \{x_1, x_2, \dots, x_5\}$ , and (ii) a weighted covering  $(T_1, T_2)$  of  $\mathcal{N}$ .

 $u'_i$  as zero for all *i*. All other arcs of  $T_1$  keep the weighting inherited from  $\mathcal{N}$ . Similarly, let  $T_2$  be the connecting subtree for X in  $\mathcal{N}$  obtained from  $\mathcal{N}$  by deleting  $(u_i, v_i)$  for all *i*, and re-weighting each arc not on the (unique) path from  $s_i$  to  $v_i$  via  $u'_i$  as zero for all *i*. We call  $(T_1, T_2)$  a weighted covering of  $\mathcal{N}$ . To illustrate this construction, an example is given in Fig. 3, where  $\mathcal{N}$  is a level-1 network, and  $(T_1, T_2)$  is a weighted covering of  $\mathcal{N}$ .

The following proposition is sufficient to show that MAX-ALLPATHS PD is polynomial time for the class of level-1 networks. The reason for this sufficiency is given after its proof.

**Proposition 4.5.** Let  $\mathcal{N}$  be a level-1 network on X, and let  $(T_1, T_2)$  be a weighted covering of  $\mathcal{N}$ . If  $S \subseteq X$ , then AllPaths-PD $_{\mathcal{N}}(S)$  equates to the sum of  $PD_{T_1}(S)$  and  $PD_{T_2}(S)$ .

**Proof.** Let  $A^{>0}(T_1)$  and  $A^{>0}(T_2)$  denote the arcs of  $T_1$  and  $T_2$ , respectively, of non-zero weight. For each  $i \in \{1, 2\}$ , let  $\phi_i$  denote the embedding map from  $A^{>0}(T_i)$  to the arc set of  $\mathcal{N}$ . By construction, for each i, the map  $\phi_i$  is one-to-one and, for each non-zero weighted arc e of  $\mathcal{N}$ , the arc e is in the co-domain of exactly one of  $\phi_1$  and  $\phi_2$ . Now suppose that  $S \subseteq X$ , and let  $\ell \in S$  and let e be a non-zero weighted arc of  $\mathcal{N}$ . Then e is on a directed path from the root of  $\mathcal{N}$  to  $\ell$  if and only if there is a unique i such that  $\phi_i^{-1}(e)$  has non-zero weight and  $\phi_i^{-1}(e)$  is on the (unique) path in  $T_i$  from its root to  $\ell$ . It now follows that

AllPaths-PD<sub>$$\mathcal{N}$$</sub>(S) = PD<sub>T1</sub>(S) + PD<sub>T2</sub>(S).  $\Box$ 

As an example of Proposition 4.5, consider Fig. 3 and choose  $S = \{x_2, x_4\}$ . Then AllPaths-PD<sub>N</sub>(S) = 16, PD<sub>T1</sub>(S) = 11, and PD<sub>T2</sub>(S) = 5. In particular,

AllPaths-PD<sub>$$\mathcal{N}$$</sub>(S) = PD <sub>$T_1$</sub> (S) + PD <sub>$T_2$</sub> (S).

Let  $\mathcal{N}$  be a level-1 network. It is clear that a weighted covering  $(T_1, T_2)$  of  $\mathcal{N}$  can be constructed in time polynomial in the size of  $\mathcal{N}$  using the approach described prior to Proposition 4.5. However, as  $\mathcal{N}$  is tree-child, the number of vertices, and thus arcs, in  $\mathcal{N}$  is linear in the size of X [6,14], and so this construction can be done in time polynomial in the size of X. By Proposition 4.5, finding the maximum value of AllPaths-PD $_{\mathcal{N}}(S)$  over all subsets S of X of size k is equivalent to finding the maximum value of PD $_{T_1}(S) + PD_{T_2}(S)$  over all subsets S of X of size k. The latter problem, called WEIGHTED AVERAGE PD on 2 TREES, is shown to be solvable in time polynomial in the size of X in [3] by reformulating the problem as a set of |X| minimum-cost flow problems. It follows that MAX-ALLPATHS-PD for the class of level-1 networks is also polynomial time in the size of X. In particular, we have the following corollary.

**Corollary 4.6.** Let  $\mathcal{N}$  be a level-1 network on X, and let k be a positive integer. Then MAX-ALLPATHS-PD( $\mathcal{N}, k$ ) can be solved in time polynomial in the size of X.

### 5. Network-PD

In this section, we turn to Network-PD, our variant of PD for phylogenetic networks that is potentially more realistic than AllPaths-PD discussed previously, but that requires additional information in the form of inheritance proportions on

each reticulation arc. Let  $\mathcal{N}$  be a phylogenetic network on X with an additional weight p(e), the inheritance proportion, on each incoming arc to each reticulation. This additional weight indicates the proportion of features of the parent vertex present in the child vertex of that arc. Recall that, for any subset  $S \subseteq X$ , we defined Network-PD $_{\mathcal{N}, p}(S)$  as

Network-PD<sub>$$\mathcal{N}, p$$</sub>(S) =  $\sum_{e \in \mathcal{N}} \gamma(S, e) \cdot w(e)$ ,

where, for each arc  $e = (u, v) \in \mathcal{N}$ , the coefficient  $\gamma(S, e)$  denotes the proportion of the features of v that are present in the taxa set S. Thus, while AllPaths-PD implicitly assumes that each reticulation inherits all features present in both its parents, Network-PD allows us to model the fact that a reticulation representing, for example, a true hybridisation event might inherit only a proportion of features from each of its two parents.

In the following corollary of Theorems 4.1 and 4.2, we observe that Network-PD is a generalisation of AllPaths-PD, from which it follows that maximising Network-PD is NP-hard.

**Corollary 5.1.** The problem MAX-NETWORK-PD is NP-hard even when the inputted phylogenetic network is restricted to be from the class of normal networks. Moreover, MAX-NETWORK-PD cannot be approximated in polynomial time with approximation ratio better than  $1 - \frac{1}{e}$  unless P = NP.

**Proof.** Given an input  $(\mathcal{N}, k)$  for Max-ALLPATHS-PD, we define an instance of Max-NETWORK-PD as  $(\mathcal{N}, p, k)$  where p(e) = 1 for all reticulation arcs. Since, for all subsets  $S \subseteq X$ , AllPaths-PD $_{\mathcal{N}}(S) =$  Network-PD $_{\mathcal{N}, p}(S)$ , both problems have the same optimal solution. As Max-ALLPATHS-PD is NP-hard, it follows that Max-NETWORK-PD is also NP-hard and, by Theorem 4.1, cannot be approximated in polynomial time with approximation ratio better than  $1 - \frac{1}{e}$  unless P = NP.  $\Box$ 

For a fixed arc *e* and a subset *A* of *X*, let  $\mathcal{E}_A$  be the event that a feature arising on arc *e* is inherited by some taxon in set *A*. Then  $\gamma(A, e) = \Pr[\mathcal{E}_A]$ . For two subsets *A*,  $B \subseteq X$ , by the inclusion-exclusion principle

$$\gamma(A \cup B, e) = \Pr[\mathcal{E}_A \cup \mathcal{E}_B] = \Pr[\mathcal{E}_A] + \Pr[\mathcal{E}_B] - \Pr[\mathcal{E}_A \cap \mathcal{E}_B] \le \gamma(A, e) + \gamma(B, e) - \gamma(A \cap B, e),$$

where the inequality is because  $\mathcal{E}_{A \cap B}$  is a sub-event of  $(\mathcal{E}_A \cap \mathcal{E}_B)$ . Thus  $\gamma$  is submodular. As for AllPaths-PD, we therefore obtain the following immediate corollary.

**Corollary 5.2.** A greedy algorithm returns a  $1 - \frac{1}{e}$  approximation for MAX-NETWORK-PD. Moreover, this approximation ratio cannot be improved unless  $P \neq NP$ .

**Remark.** We have already seen that the case of MAX-NETWORK-PD in which p(e) = 1 on all reticulation arcs is equivalent to MAX-ALLPATHS-PD and is NP-hard. It is also the case that if p(e) = 0.5 on all reticulation arcs (which might correspond to each reticulation being a perfect hybrid), then MAX-ALLPATHS-PD is NP-hard. This can be seen by a reduction from the NP-complete problem EXACT-COVER-BY-4-SETS, which takes as input a set *E* with |E| = 4q, and a collection *C* of 4-element subsets of *E* with no element occurring in more than four subsets. The objective is to decide if there is a subset *C'* of *C* which is a partition of *E*. Such a subset is called an *exact cover*. The construction is similar to that shown in Fig. 2, where the leaf set is *C*, and there is an exact cover if and only if the optimal Network-PD of a subset of |E|/4 leaves is |E|/4 (each leaf contributing four weight-1 arcs but with  $\gamma$  averaging 0.25).

### 5.1. Max and Min Network-PD

In the previous section, we have seen that Network-PD is a generalisation of AllPaths-PD obtained by setting the inheritance proportion p(e) to one for each reticulation arc e of a phylogenetic network  $\mathcal{N}$ . If we restrict the inheritance proportions such that, for a reticulation with incoming arcs  $e_1$  and  $e_2$  to

$$p(e_1) + p(e_2) = 1$$
,

we obtain the following relationship between the maximum (respectively, minimum) value of Network-PD and MaxWeight-Tree-PD (respectively, MinWeightTree-PD) as defined in Section 3.

**Theorem 5.3.** Let  $\mathcal{N}$  be a phylogenetic network on X, and let S be a fixed subset of k elements of X. Let R be the set of reticulation arcs of  $\mathcal{N}$ , and let P be the set of all functions mapping R to  $[0, 1]^{|R|}$  with the restriction that at each reticulation the incoming arcs,  $e_1, e_2$  say, have inheritance proportions adding up to 1, that is  $p(e_1) + p(e_2) = 1$ . Then

$$\max_{p \in P} \text{Network-PD}_{\mathcal{N}, p}(S) = \text{MaxWeightTree-PD}_{\mathcal{N}}(S).$$

and

 $\min_{p \in P} \text{Network-PD}_{\mathcal{N}, p}(S) = \text{MinWeightTree-PD}_{\mathcal{N}}(S).$ 

**Proof.** We prove the maximisation part of the theorem. The proof of the minimisation part is similar and omitted. Let *T* be a connecting subtree for *S* in  $\mathcal{N}$  such that  $PD_T(S) = MaxWeightTree-PD_{\mathcal{N}}(S)$ . Let  $p_{max}$  be a function on *R* defined as follows: at each reticulation *v* of  $\mathcal{N}$  that is in *T*, set  $p_{max}(e) = 1$  if *e* is directed into *v* and *e* is in *T* and set  $p_{max}(e) = 0$  if *e* is directed into *v* and *e* is not in *T*, and at each reticulation of  $\mathcal{N}$  that is not in *T*, set  $p_{max}$ , all features are inherited along the arcs of *T* and hence

$$\max_{p \in P} \text{Network-PD}_{\mathcal{N}, p}(S) \ge \text{Network-PD}_{p_{\text{max}}}(S) = \text{MaxWeightTree-PD}(S).$$

Now consider  $p_0 \in P$  which maximises Network-PD<sub> $N, p_0$ </sub>(S) and among all p which maximise Network-PD<sub>N, p</sub>(S), choose  $p_0$  to have a minimum number of arcs e with fractional inheritance proportion, i.e. such that  $p_0(e) \notin \{0, 1\}$ . Suppose that for all reticulation arcs e, we have  $p_0(e) \in \{0, 1\}$ . Then at every reticulation one incoming arc has  $p_0$  equal to 1 and the other has  $p_0$  equal to 0. Therefore Network-PD<sub>N, p</sub>(S) is the PD of the minimal connecting tree of S in the tree obtained from N by deleting all reticulation arcs of N with  $p_0$  equal to 0, and so

$$\max_{p \in P} \text{Network-PD}_{\mathcal{N}, p}(S) = \text{Network-PD}_{\mathcal{N}, p_0}(S) \le \text{MaxWeightTree-PD}_{\mathcal{N}}(S).$$

This proves the maximisation part of the theorem unless there is some arc with  $p_0 \notin \{0, 1\}$ .

Now suppose, for a contradiction, that there is some reticulation arc with  $p_0 \notin \{0, 1\}$ . Then there must be a reticulation v with parents  $u_1, u_2$  such that (i)  $p_0(u_1), p_0(u_2) \notin \{0, 1\}$ , (ii) for all reticulations that are descendants of v the incoming arcs have  $p_0$  equal to 0 or 1, and (iii) there is a subset  $S' \subseteq S$  such that there is a path from v to each element of S' consisting of tree arcs and reticulation arcs with  $p_0 = 1$ . (Otherwise we can follow arcs down towards leaves until we find a last reticulation with inheritance from both parents, and if it is not an ancestor of any leaf in S, then we can reset its incoming arcs weights without affecting Network-PD(S), thereby reducing the number of reticulations with positive inheritance from both parents.)

Now consider the contribution to Network-PD<sub> $N, p_0$ </sub>(*S*) of each arc *e* in N. This is *w*(*e*) times the probability that a feature that arises on *e* is inherited by some member of *S*, where the only randomness comes on reticulations which have  $p_0 \notin \{0, 1\}$ . For all subsets  $A \subseteq S$ , let  $\mathcal{E}_A^e$  be the event that a feature that arises on *e* is inherited by an element of *A*. Then the contribution of *e* to Network-PD<sub> $N, p_0$ </sub>(*S*) is

$$w(e) \operatorname{Pr}[\mathcal{E}_{S}^{e}] = w(e) \operatorname{Pr}[\mathcal{E}_{S \setminus S'}^{e}] + w(e) \operatorname{Pr}[\overline{\mathcal{E}_{S \setminus S'}^{e}} \cap \mathcal{E}_{S'}^{e}],$$

where, as above, S' is the subset of S consisting of those elements in S that can be reached from v by paths whose reticulation arcs have  $p_0 = 1$ . Since all reticulation arcs below v have  $p_0 \in \{0, 1\}$ , it follows that if e is a descendent arc of v, then  $\Pr[\overline{\mathcal{E}^e_{S\setminus S'}} \cap \mathcal{E}^e_{S'}] = \Pr[\mathcal{E}^e_{S'}]$  and it is either 0 or 1 but, importantly, it is independent of  $p_0((u_1, v))$  and  $p_0((u_2, v))$ .

Let  $\mathcal{E}_{u_1}^e$  be the event that a feature that arises on *e* is inherited down to the vertex  $u_1$ , and  $\mathcal{E}_{u_2}^e$  be the event that a feature that arises on *e* is inherited down to the vertex  $u_2$ . If *e* is not a descendant arc of *v*, then writing  $q_0 = p_0((u_1, v))$ , and so  $(1 - q_0) = p_0((u_2, v))$ , we have

$$\Pr[\overline{\mathcal{E}^{e}_{S\setminus S'}} \cap \mathcal{E}^{e}_{S'}] = \Pr[\overline{\mathcal{E}^{e}_{S\setminus S'}} \cap \mathcal{E}^{e}_{u_1}]q_0 + \Pr[\overline{\mathcal{E}^{e}_{S\setminus S'}} \cap \mathcal{E}^{e}_{u_2}](1-q_0) - \Pr[\overline{\mathcal{E}^{e}_{S\setminus S'}} \cap \mathcal{E}^{e}_{u_1} \cap \mathcal{E}^{e}_{u_2}]q_0(1-q_0).$$

So the full contribution from all arcs not descendants of v is

$$\sum_{e} w(e) \left( \Pr[\mathcal{E}^{e}_{S \setminus S'}] + \Pr[\overline{\mathcal{E}^{e}_{S \setminus S'}} \cap \mathcal{E}^{e}_{u_{1}}]q_{0} + \Pr[\overline{\mathcal{E}^{e}_{S \setminus S'}} \cap \mathcal{E}^{e}_{u_{2}}](1-q_{0}) - \Pr[\overline{\mathcal{E}^{e}_{S \setminus S'}} \cap \mathcal{E}^{e}_{u_{1}} \cap \mathcal{E}^{e}_{u_{2}}]q_{0}(1-q_{0}) \right)$$

For convenience, write  $A = \sum_{e} w(e) \Pr[\mathcal{E}^{e}_{S \setminus S'}]$ ,  $B = \sum_{e} w(e) \Pr[\overline{\mathcal{E}^{e}_{S \setminus S'}} \cap \mathcal{E}^{e}_{u_{1}}]$ ,  $C = \sum_{e} w(e) \Pr[\overline{\mathcal{E}^{e}_{S \setminus S'}} \cap \mathcal{E}^{e}_{u_{2}}]$ , and  $D = \sum_{e} w(e) \Pr[\overline{\mathcal{E}^{e}_{S \setminus S'}} \cap \mathcal{E}^{e}_{u_{1}} \cap \mathcal{E}^{e}_{u_{2}}]$ . Note that  $D \leq \min\{B, C\}$ . Without loss of generality, we may assume that  $B \geq C$ . Then we get the contribution to Network-PD<sub>N, p\_0</sub>(S) from all arcs not descendants of v is

$$A + Bq_0 + C(1 - q_0) - Dq_0(1 - q_0) < A + B$$

Hence if we amend  $p_0$  by setting  $p_0((u_1, v)) = q_0 = 1$  and  $p_0((u_2, v)) = 0$ , then we can only be increasing Network-PD<sub> $N, p_0(S)$ </sub> and, simultaneously, reducing the number of arcs *e* such that  $p_0(e) \notin \{0, 1\}$ . This contradicts the choice of  $p_0$ , and hence it must be that there is no arc with  $p_0 \notin \{0, 1\}$ . This completes the proof of the theorem.  $\Box$ 

Theorem 5.3 gives us the following immediate corollary.

**Corollary 5.4.** Let  $\mathcal{N}$  be a phylogenetic network on X, let k be a positive integer, and let P be the set of all inheritance proportion functions whereby, if  $p \in P$ , and  $e_1$  and  $e_2$  are the reticulation arcs directed into a reticulation of  $\mathcal{N}$ , then  $p(e_1) + p(e_2) = 1$ . Then

 $\max_{p \in P} \text{Max-Network-PD}(\mathcal{N}, p, k) = \text{Max-MaxWeightTree-PD}(\mathcal{N}, k)$ 

and

 $\min_{p \in P} \text{Max-Network-PD}(\mathcal{N}, p, k) = \text{Max-MinWeightTree-PD}(\mathcal{N}, k).$ 

# 6. MaxWeightTree-PD

Given the importance of MaxWeightTree-PD and MinWeightTree-PD as bounds for Network-PD, we now analyse the complexity of determining the maximum possible PD score over all subsets of taxa of size k under these two variants more in-depth. We begin by considering MaxWeightTree-PD and turn to MinWeightTree-PD in Section 7.

Let  $\mathcal{N}$  be a phylogenetic network on X. Recall that, for any subset  $S \subseteq X$ , we have defined MaxWeightTree-PD(S) to be the maximum of  $\sum_{e \in T} w(e)$  over all connecting subtrees for S in  $\mathcal{N}$ . We now show that the corresponding optimisation problem Max-MaxWeightTree-PD can be solved in polynomial time by reducing Max-MaxWeightTree-PD to a minimumcost flow problem, following the approach of [3].

**Theorem 6.1.** Let N be a phylogenetic network on X, and let k be a positive integer. Then MAX-MAXWEIGHTTREE-PD applied to N and k can be solved in polynomial time.

**Proof.** Starting with  $\mathcal{N}$ , we define a flow network by

- setting the root  $\rho$  of  $\mathcal N$  to be the source,
- adding additional arcs from  $\rho$  to each tree vertex of N, which we shall call the *extra arcs*,
- appending a new vertex *t* with an arc from each leaf of N directed into *t*, and a new vertex *t'*, the sink, with a single arc from *t* to *t'*,
- setting the capacity of all arcs inherited from N, and the arcs from the leaves to t, to be 1,
- setting the capacity of the extra arcs and the final arc (t, t') to be k, and
- setting the cost of each arc *e* inherited from N to be the negative of its weight, that is -w(e), and the cost of all the additional arcs to be 0.

An example for this construction is given in Fig. 4. Observe that, due to the arc (t, t'), the maximum flow from the source  $\rho$  to the sink t' is k units. Therefore, as all capacities are integral, there is a minimum-cost integral flow of k units that may be found in polynomial time (see, for example, [1,3]).

Since there is a cut of the flow network between the leaves in  $\mathcal{L}(\mathcal{N})$  and t, and each of these arcs has capacity 1, exactly k of these arcs are used in the minimum-cost integral flow. We denote the set of leaves adjacent to these arcs by S. Note that if a minimum-cost flow has non-zero flow through any extra arc  $(\rho, v)$ , then there is a minimum-cost flow that has non-zero flow in the arc (u, v) of  $\mathcal{N}$  directed into v, since there is a path from  $\rho$  to v via (u, v) which has lower cost than the path from  $\rho$  to v via the extra arc  $(\rho, v)$  and is not at capacity due to the extra arcs. (In the case that the arc (u, v) has weight zero, this path actually has the same cost but, without loss of generality, we can still assume our minimum-cost flow routes through (u, v).)

Therefore the set of arcs of  $\mathcal{N}$  that have non-zero flow form a connecting subtree  $T_S$  for S, since (i), by the argument of the previous paragraph, there must be flow from the root to each leaf in S and (ii), each arc directed out of a reticulation has capacity 1, so at most one incoming arc to a reticulation has non-zero flow. The total cost of such a flow is exactly the negative of the sum of the weight of arcs in the  $T_S$ . Moreover, any connecting subtree  $T_S$  for S can be realised as a flow of k units by routing as much flow as possible through the arcs constituting  $T_S$ , and routing extra flow through the extra arcs as necessary. Since we can find the minimum-cost integral k-flow in polynomial time, we can therefore find the max-weight embedded connecting subtree for any set of k leaves of  $\mathcal{N}$  in polynomial time.  $\Box$ 

**Remark.** The proof of the last theorem can be easily extended to show that the MaxWeightTree-PD can be optimised for the following problem using a construction similar to that used in [3] for the analogous optimisation problem for phylogenetic trees.

#### WEIGHTED AVERAGE PD ON 2 NETWORKS

**Input:** Two phylogenetic networks  $N_1$  and  $N_2$  on X with (arc) weight functions  $w_1$  and  $w_2$ , and a positive integer k. **Objective:** Determine the maximum value of

$$\sum_{e\in T_1} w_1(e) + \sum_{e\in T_2} w_2(e),$$

where  $T_1 \in \mathsf{T}_S(\mathcal{N}_1)$  and  $T_2 \in \mathsf{T}_S(\mathcal{N}_2)$ , over all subsets  $S \subseteq X$  of cardinality *k*.



**Fig. 4.** (i) Phylogenetic network  $\mathcal{N}$  on  $X = \{x_1, \dots, x_6\}$  (identical to the phylogenetic network  $\mathcal{N}$  shown in Fig. 1). (ii) The flow network resulting from the construction described in the proof of Theorem 6.1. Each solid arc has the indicated cost and capacity 1. The dotted arcs have cost 0 and capacity k.

# 7. MinWeightTree-PD

Recall that, for a phylogenetic network on *X*, we defined MAX-MINWEIGHTTREE-PD to be the problem of determining the maximum weight, over all subsets of *X* of cardinality *k*, of the minimum weight connecting subtree of the subset. Our first observation is that for an arbitrary phylogenetic network  $\mathcal{N}$  on *X*, even computing MinWeightTree-PD<sub> $\mathcal{N}$ </sub>(*X*) is computationally hard. To make this more precise consider the following problem:

### **MINIMUM-WEIGHT** X-**TREE** $(\mathcal{N})$

**Input:** A phylogenetic network  $\mathcal{N}$  on taxa set X. **Objective:** The value of MinWeightTree-PD<sub> $\mathcal{N}$ </sub>(X), i.e. the minimum weight of a connecting subtree for X in  $\mathcal{N}$ .

We will show that this problem is hard by making use of a reduction from the well-known NP-complete problem Exact Cover By 3-SETS [12]:

#### **EXACT COVER BY 3-SETS**(X, C)

**Input:** A set *X* with |X| = 3q, and a collection *C* of 3-element subsets of *X* with no element occurring in more than three subsets.

**Objective:** Determine if *C* contains an exact cover of *X*, that is a subset *C'* of *C* which is a partition of *X*?

**Theorem 7.1.** *The problem MINIMUM-WEIGHT X-TREE is NP-hard.* 

**Proof.** Take an instance of EXACT COVER BY 3-SETS:, i.e. a set *X* with |X| = 3q, and a collection  $C = \{C_1, C_2, ..., C_k\}$  of 3-element subsets of *X* with no element occurring in more than three subsets. Similar to a construction in [12], construct a phylogenetic network on *X* as follows. Let *D* be the rooted acyclic digraph with vertex set  $C \cup X \cup \rho$  and arc set

$$\{(\rho, C_i) : i \in \{1, 2, \dots, k\}\} \cup \{(C_i, x) : x \in X \cap C_i\}.$$

Now weight the arcs of D so that  $(\rho, C_i)$  has weight 3 for all i and all remaining arcs have weight zero. We next construct a phylogenetic network  $\mathcal{N}$  on X from D and its weighting. First, refine the vertices  $\rho$  and  $C_i$  for all i so that all vertices (except elements of X) with in-degree zero or in-degree one have out-degree two. Second, for each element x in X, adjoin a new vertex to it via a new arc so that the new vertex has in-degree one (and out-degree zero) and relabel so that the resulting new vertex is now x. Third, refine each vertex with in-degree three so that no vertex has in-degree more than two. Lastly, extend the weighting of D by assigning all (new) unweighted arcs weight zero. The resulting phylogenetic network on X is  $\mathcal{N}$ . To illustrate the construction, the top half of D and its weighting, and a possible top half of  $\mathcal{N}$  is shown in Fig. 5(i) and (ii), respectively. Clearly,  $\mathcal{N}$  can be constructed in time polynomial in the size of the initial instance of Exact COVER BY 3-SETS. Furthermore, it is easily seen that C contains an exact cover of X if and only if  $\mathcal{N}$  has a connecting subtree for X of weight at most |X|. Hence computing MinWeightTree-PD $_{\mathcal{N}}(X)$  is NP-hard.  $\Box$ 

Although we have shown that computing MinWeightTree-PD<sub> $\mathcal{N}$ </sub>(*X*) is hard on a general phylogenetic network  $\mathcal{N}$ , if we restrict  $\mathcal{N}$  to be a tree-child network, the problem of computing MinWeightTree-PD<sub> $\mathcal{N}$ </sub>(*X*) can be solved in polynomial time.



**Fig. 5.** (i) The top half of *D* and its weighting, and (ii) a possible top half of  $\mathcal{N}$ .

**Theorem 7.2.** Let N be a tree-child network on X. Then MINIMUM-WEIGHT X-TREE applied to N can be solved in polynomial time in the size of X.

**Proof.** Let *T* be a connecting subtree for *X* in  $\mathcal{N}$ . Since  $\mathcal{N}$  is tree-child, *T* contains every tree arc of  $\mathcal{N}$  and *T* contains, for each reticulation *v* of  $\mathcal{N}$ , precisely one reticulation arc directed into *v* [25]. Thus, to find a minimum-weight connecting subtree for *X* in  $\mathcal{N}$  it suffices to determine for each reticulation *v<sub>i</sub>*, a reticulation arc of minimum weight directed into *v<sub>i</sub>*. In particular, if *e<sub>i</sub>* is such an arc for all *i*, then the arc set of a minimum-weight connecting subtree for *X* in  $\mathcal{N}$  is the union of the set of tree arcs in  $\mathcal{N}$  and {*e<sub>i</sub>* : *v<sub>i</sub>* is a reticulation in  $\mathcal{N}$ }. This completes the proof of the theorem.  $\Box$ 

In contrast to the last theorem, computing MinWeightTree-PD<sub> $\mathcal{N}$ </sub>(*S*) for a *given* subset *S*  $\subset$  *X* of a phylogenetic network  $\mathcal{N}$  on *X* is hard even if  $\mathcal{N}$  is a normal network (and so, in particular, if  $\mathcal{N}$  is tree-child).

**Theorem 7.3.** Let  $\mathcal{N}$  be a phylogenetic network on X and let  $S \subset X$  be a strict subset of X. Then, computing MinWeightTree-PD<sub> $\mathcal{N}$ </sub>(S) is NP-hard even if  $\mathcal{N}$  is a normal network.

**Proof.** Take an instance of MINIMUM-WEIGHT X-TREE, i.e. an arbitrary phylogenetic network  $\mathcal{N}$  on X. We construct a normal network  $\mathcal{N}'$  on  $X' \supset X$  from  $\mathcal{N}$  by subdividing all reticulation arcs and adjoining a new leaf via a new arc to each new vertex. If (u, v) was a reticulation arc in  $\mathcal{N}$  with weight w(u, v), we assign weight w(u, v) to the arc of the subdivision directed into the corresponding reticulation in  $\mathcal{N}'$ , and we assign weight zero to the other arc of the subdivision as well as to the incident pendant arc leading to a new leaf in X' - X. Setting  $S = X \subset X'$ , the problem of calculating MinWeightTree-PD $_{\mathcal{N}'}(S)$  for the normal network  $\mathcal{N}'$  on X' corresponds to the problem of calculating MinWeightTree-PD $_{\mathcal{N}'}(S)$  for the normal network  $\mathcal{N}'$  on X' and  $S \subset X'$  is NP-hard. This completes the proof of the theorem.  $\Box$ 

We now turn to the original problem of this section and show that it is again an NP-hard problem.

# Theorem 7.4. The problem MAX-MINWEIGHTTREE-PD is NP-hard.

**Proof.** Take an instance of MINIMUM-WEIGHT X-TREE, i.e. a phylogenetic network  $\mathcal{N}$  on X with |X| = k. We now construct a phylogenetic network  $\mathcal{N}'$  on  $X' \supset X$  as follows:

- Choose a pendant arc *e* leading to a leaf, say *x*, of N, subdivide it (possibly several times), and adjoin a new leaf via a new arc with weight zero to each new vertex.
- If the weight of e in  $\mathcal{N}$  was w(e), assign weight w(e) to the arc incident with x, and assign weight zero to all other arcs of the subdivision.

Now, consider the instance  $(\mathcal{N}', k)$  of the problem MAX-MINWEIGHTTREE-PD, i.e. consider the problem of computing the maximum value of MinWeightTree-PD<sub> $\mathcal{N}'$ </sub>(*S*) over all subsets  $S \subseteq X'$  of cardinality |X| = k on  $\mathcal{N}'$ . As all elements in X' - X are attached to  $\mathcal{N}'$  via pendant arcs of weight zero and all non-pendant arcs on a path from the root of some connecting subtree *T* for X' in  $\mathcal{N}$  to elements in X' - X are also covered by a path from the root of *T* to *x*, there is a subset  $S \subseteq X'$  of cardinality k = |X| maximising MinWeightTree-PD<sub> $\mathcal{N}'$ </sub>(*S'*) over all subsets  $S' \subseteq X'$  with |S'| = |X| that does not contain any of the leaves in X' - X. In other words, we can assume that S = X. Thus, the maximum value of MinWeightTree-PD<sub> $\mathcal{N}'$ </sub>(*S'*) in  $\mathcal{N}'$  over all subsets  $S' \subseteq X'$  with |S'| = |X| coincides with the value of MinWeightTree-PD<sub> $\mathcal{N}(X)$ </sub> in  $\mathcal{N}$ . By Theorem 7.1, the latter problem is NP-hard, and so we conclude that the problem MAX-MINWEIGHTTREE-PD is also NP-hard.  $\Box$ 



**Fig. 6.** (i) Semi-binary level-1 network  $\mathcal{N}$ , and (ii) a possible resolution into a binary level-1 network  $\mathcal{N}'$ . In the network  $\mathcal{N}$ , the tree vertex u is the source of reticulations  $v_1$  and  $v_2$ , and the arcs incident with u "leading to"  $v_1$ , respectively  $v_2$ , are  $e_1$  and  $e'_1$ , respectively  $e_2$  and  $e'_2$ . In the resolution  $\mathcal{N}'$ , these pairs of arcs are incident to the same tree vertex, respectively. Moreover, all arcs of  $\mathcal{N}'$  inherit their weights from  $\mathcal{N}$ , and the three newly added arcs are assigned weight 0.

### 8. Semi-binary phylogenetic networks

We have presented the arguments in this paper in terms of binary phylogenetic networks, both for simplicity of understanding and because the hardness results are stronger. In this section, we discuss extending the results to so-called *semi-binary* phylogenetic networks [5]. The definition of a semi-binary phylogenetic network is the same as for a binary phylogenetic network except that non-leaf vertices of in-degree one are allowed to have out-degree at least two. Naturally, such vertices are called *tree vertices*. First note that all hardness results (Theorems 4.1, 4.2, 7.3, 7.4 and Corollary 5.1) hold for semi-binary phylogenetic networks, since binary phylogenetic networks are a special case of such phylogenetic networks.

Given any semi-binary phylogenetic network  $\mathcal{N}$  on X in which there are tree vertices of degree greater than two, we can resolve such vertices arbitrarily, inserting new arcs assigned weight 0, and obtain a binary phylogenetic network  $\mathcal{N}'$  on X such that the PD of any subset  $S \subseteq X$  is the same on  $\mathcal{N}$  and  $\mathcal{N}'$ , under any of the variants we have discussed. Thus Corollary 4.4 and Theorem 6.1 hold for semi-binary phylogenetic networks. However, this is not quite enough to ensure that all of the positive results in the paper also hold for semi-binary phylogenetic networks as some have additional conditions, in particular, the binary phylogenetic network is either level-1 or tree-child. Consequently, we must both define these properties for semi-binary networks, and ensure that we can resolve  $\mathcal{N}$  so that these properties are preserved in  $\mathcal{N}'$ .

A semi-binary phylogenetic network is *tree-child* if each non-leaf vertex is the parent of a tree vertex or a leaf. Let  $\mathcal{N}$  be a semi-binary tree-child network, and suppose that u is a tree vertex of  $\mathcal{N}$  with out-degree more than two. Let v be a child of u that is also a tree vertex. We now describe a construction that iteratively resolves  $\mathcal{N}$  to a binary tree-child network. Let  $u_1, u_2, \ldots, u_k$  denote the children of u other than v. Next, subdivide (u, v) with vertices  $w_1, w_2, \ldots, w_{k-1}$  and, for each  $i \in \{1, 2, \ldots, k-1\}$ , delete  $(u, u_i)$  and join  $w_i$  and  $u_i$  with the new arc  $(w_i, u_i)$ . Noting that the unique path from u to v consists of tree vertices, it follows that, as  $\mathcal{N}$  is tree-child, the resulting semi-binary phylogenetic network  $\mathcal{N}'$  is also tree-child. Iteratively resolving each of the tree vertices of  $\mathcal{N}'$  with out-degree more than two in the same way gives a binary tree-child network. Thus, Theorem 7.2 holds for semi-binary tree-child networks.

A semi-binary phylogenetic network is a *level-1 network* if all of its biconnected components contain at most one reticulation vertex. Notice that in the case of binary phylogenetic networks this definition coincides with the definition of level-1 networks presented earlier. However, in the case of semi-binary phylogenetic networks, the underlying (undirected) cycles in a level-1 network do not need to be vertex disjoint. An example is given in Fig. 6(i). Let  $\mathcal{N}$  be a semi-binary level-1 network, and suppose that u is a tree vertex of  $\mathcal{N}$  with out-degree more than two. Since  $\mathcal{N}$  is level-1, observe that if u is a vertex in k distinct underlying cycles of  $\mathcal{N}$ , where  $k \ge 2$ , then u is the source vertex of at least k - 1 reticulations. Now, for each tree vertex u of  $\mathcal{N}$  with out-degree more than two, resolve u so that if u is the source vertex of a reticulation v, then the two arcs incident with u that "lead to" v are incident to the same tree vertex after the resolution. It is easily seen that the resulting binary phylogenetic network is level-1. To illustrate, a semi-binary level-1 network and a possible binary resolution is given in Fig. 6. It now follows that Proposition 4.5 holds for semi-binary level-1 networks.

#### 9. Concluding remarks

Phylogenetic diversity is widely used for quantifying the biodiversity of a set of species based on their evolutionary history and relatedness. Traditionally, PD was calculated on a phylogenetic tree representing the evolution of a set of species. However, it is now commonly accepted that evolution is not always tree-like and that many species' evolutionary history contains reticulation events such as hybridisation or lateral gene transfer. In this paper, we therefore defined four natural variants of the PD score for a subset of taxa whose evolutionary history is represented by a phylogenetic network. Under these variants, we considered the computational complexity of, given a positive integer k, determining the maximum PD score over all subsets of taxa of size k when the input is restricted to different classes of phylogenetic networks. More

precisely, we showed that determining the maximum PD score over all subsets of taxa of size k under AllPaths-PD is NPhard even when the inputted phylogenetic network is restricted to be from the class of normal networks. However, the problem is solvable in polynomial time for the class of level-1 networks. The corresponding maximisation problem is also NP-hard under Network-PD and MinWeightTree-PD (again, even when the inputted phylogenetic network is restricted to be from the class of normal networks), but it is solvable in polynomial time under MaxWeightTree-PD.

An interesting question, however, is to determine the computational complexity of the problems MAX-NETWORK-PD and MAX-MINWEIGHTTREE-PD when the inputted phylogenetic network is restricted to be from the class of level-1 networks. We leave this problem to future research.

#### **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.

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