Phylogenetic diversity and biodiversity indices on phylogenetic networks

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Abstract

In biodiversity conservation it is often necessary to prioritize the species to conserve. Existing approaches to prioritization, e.g. the Fair Proportion Index and the Shapley Value, are based on phylogenetic trees and rank species according to their contribution to overall phylogenetic diversity. However, in many cases evolution is not treelike and thus, phylogenetic networks have come to the fore as a generalization of phylogenetic trees, allowing for the representation of non-treelike evolutionary events, such as horizontal gene transfer or hybridization. Here, we extend the concepts of phylogenetic diversity and phylogenetic diversity indices from phylogenetic trees to phylogenetic networks. On the one hand, we consider the treelike content of a phylogenetic network, e.g. the (multi)set of phylogenetic trees displayed by a network and the LSA tree associated with it. On the other hand, we derive the phylogenetic diversity of subsets of taxa and biodiversity indices directly from the internal structure of the network. Furthermore, we introduce our software package NetDiversity, which was implemented in Perl and allows for the calculation of all generalized measures of phylogenetic diversity and generalized phylogenetic diversity indices established in this note.

We apply our methods to a phylogenetic network representing the evolutionary relationships among swordtails and platyfishes (Xiphophorus: Poeciliidae), a group of species characterized by widespread hybridization.

Keywords: Hybridization, Phylogenetic networks, Phylogenetic diversity, Shapley Value, Fair Proportion Index

1. Introduction

Facing a major extinction crisis and the inevitable loss of biodiversity at the same time with limited financial means, biological conservation has to prioritize the species to conserve. In this matter, the so-called phylogenetic diversity

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Faith (1992) has been introduced as a measure of biodiversity based on the evolutionary history of species. It serves as a basis for biodiversity indices used in taxon prioritization, e.g. the Fair Proportion Index and the Shapley Value (Hanke et al. (2007); Hartmann (2013); Fuchs and Jin (2015); Wicke and Fischer (2017)).

Both phylogenetic diversity, as well as the Fair Proportion Index and the Shapley Value are based on phylogenetic trees and thus, assume the evolutionary history of species to be treelike. However, there are several forms of non-treelike evolution, such as horizontal gene transfer or hybridization, affecting a variety of species. Therefore, phylogenetic reticulation networks have become an important concept in evolutionary biology, allowing for the representation of non-treelike evolution.

Here, we aim at combining both approaches, i.e. we aim at extending the concept of phylogenetic diversity and its measures from phylogenetic trees to phylogenetic networks. So far, phylogenetic diversity and the Shapley Value have been considered for so-called split networks, which can be used to represent conflict in data (Chernomor et al. (2016); Volkmann et al. (2014)), but no attempts have been made towards the generalization of phylogenetic diversity and its measures to reticulation networks.

In this note we first recapitulate phylogenetic diversity, the Fair Proportion Index and the Shapley Value on phylogenetic trees, before we focus on generalizing these concepts to phylogenetic networks.

We will introduce a variety of definitions for generalized phylogenetic diversity, following three main principles: the calculation of spanning arborescences and subgraphs of a network, the consideration of the (multi)set of phylogenetic trees displayed by a network and the construction of the so-called LSA tree associated with a network.

We will then turn our attention to the Fair Proportion Index and the Shapley Value and suggest different ways of using them as taxon prioritization tools in the context of phylogenetic networks.

All approaches are implemented in our new software tool NetDiversity, which has been made publicly available at www.mareikefischer.de/Software/NetDiversity.zip. Moreover, we test NetDiversity on a recently published phylogenetic network of swordtails and platyfishes (Xiphophorus: Poeciliidae), whose evolution is characterized by widespread hybridization (Solís-Lemus and Ané (2016)).

2. Preliminaries

Let $X$ be a finite set of species (taxa). A rooted phylogenetic $X$-tree $T$ is a rooted tree with root $\rho$ where the leaves are bijectively labeled by $X$. $T$ is called binary if all internal nodes have degree 3 and the root has degree 2. Throughout this paper, when we refer to trees, we always mean rooted phylogenetic trees. Furthermore, we assume all edges in a tree to have edge lengths greater than zero assigned to them, and we denote the length of an edge $e$ as $\lambda_e > 0$.

Note that all edges in a rooted phylogenetic tree $T$ are directed away from the root, thus formally the treeshape of $T$ is a so-called arborescence.
Definition 1 (Arborescence). Let $G = (V, E)$ be a directed graph and let $\rho \in V$ be a specified root node (of indegree 0). Then $G$ is an arborescence (rooted at $\rho$) if there is exactly one directed path from $\rho$ to $u$ for all nodes $u \in V \setminus \{\rho\}$.

A rooted binary phylogenetic network $N$ on $X$ is a connected rooted acyclic digraph such that:

- the root has outdegree 2 (and indegree 0),
- each node with outdegree 0 has indegree 1, and the set of nodes with outdegree 0 is bijectively labeled by $X$,
- all other nodes either have indegree 1 and outdegree 2, or indegree 2 and outdegree 1.

Nodes with indegree 2 and outdegree 1 are called reticulation nodes and all other nodes are called tree nodes. Furthermore, tree nodes with outdegree 0 are referred to as leaves. Edges directed into a reticulation node are called reticulation edges and edges directed into a tree node are called tree edges. When we refer to phylogenetic networks, we always mean rooted binary phylogenetic networks. Moreover, we assume all tree edges to have edge lengths greater than zero assigned to them and denote the length of a tree edge $e$ as $\lambda_e > 0$. W.l.o.g. we define the edge lengths of all reticulation edges to be zero. When we refer to the size of a tree or a network, we mean the number $n = |X|$ of taxa, i.e. the number of leaves of the tree or network under consideration.

Let $N$ be a phylogenetic network on $X$ and let $T$ be a phylogenetic $X$-tree. We say that $T$ is embedded in $N$, or that $N$ displays $T$, if $T$ can be obtained from $N$ by deleting one of the reticulation edges for each reticulation node and suppressing resulting nodes of indegree 1 and outdegree 1. We use $T(N)$ to denote the (multi)set of all rooted phylogenetic $X$-trees displayed by $N$.

Note that we receive the edge weights of an embedded tree $T \in T(N)$ as follows: for all formerly distinct edges that are melted into a new edge by suppressing nodes of indegree 1 and outdegree 1, we add their edge lengths, while all other edges keep their original weights. Moreover, note that if there are $k$ reticulation nodes in a rooted binary phylogenetic network $N$ on a taxon set $X$, then there are at most $2^k$ phylogenetic $X$-trees displayed by $N$. However, this bound does not have to be sharp (cf. Figure 1).

For a phylogenetic network $N$ and a node $u$ of $N$ that is not the root, we call any node $v$ that lies on all directed paths from the root to $u$ a stable ancestor of $u$. The so-called lowest stable ancestor of $u$ is defined as the last node $lsa(u)$ that is contained on all paths from the root to $u$, excluding $u$. Based on this terminology we can define the LSA tree (lowest stable ancestor tree) associated with a network. Let $N$ be rooted phylogenetic network on $X$. The LSA tree $T_{LSA}(N)$ associated with $N$ is a rooted phylogenetic $X$-tree that can be computed as follows: For each reticulation node $r$ in $N$, remove all edges directed into $r$ and add a new edge $e = (lsa(r), r)$ from the lowest
stable ancestor of r into r. Then repeatedly remove all unlabeled leaves and
nodes with in- and outdegree 1, until no further such removal is possible. Note
that the LSA tree associated with a binary rooted phylogenetic network is not
necessarily a binary phylogenetic tree (cf. Figure 2).
In order to use the LSA tree for subsequent phylogenetic diversity calculations,
we have to infer edge lengths for the edges of the LSA tree. For all tree edges
of N that are also present in T_{LSA}(N), we use their original edge weights. If
during the removal of nodes of in-and outdegree 1 two formerly distinct tree
eges of N are melted into a new edge in T_{LSA}(N), we add their original edge
lengths. For all newly established edges e = (lsa(r), r) between a reticulation
node r and its lowest stable ancestor, we suggest to set the length of these edges
to the average path length of a path between lsa(r) and r, respectively, i.e. we
set
\[ \lambda_{e=(lsa(r),r)} = \frac{1}{|\mathcal{P}_r|} \sum_{P \in \mathcal{P}_r} \text{length}(P), \]
where \( \mathcal{P}_r \) is the set of all lsa(r)-r-paths P in N and the length of any such path
is obtained by adding the edge lengths of all edges that are part of this path
(cf. Figure 2).

2.1. Phylogenetic diversity and phylogenetic diversity indices on trees

In this section we briefly recapitulate the concept of phylogenetic diversity
and phylogenetic diversity indices, in particular the Shapley Value and the Fair
Proportion Index, for phylogenetic trees.

**Definition 2** (Phylogenetic diversity). Let T be a rooted phylogenetic tree
with leaf set X. For a subset S \( \subseteq X \) of taxa, the phylogenetic diversity PD(S)
is calculated by summing up the edge lengths of the phylogenetic subtree of
T containing S and the root (i.e., we consider the sum of edge lengths in the
smallest spanning tree containing S and the root).
Figure 2: Rooted binary phylogenetic network \( \mathcal{N} \) on \( X = \{A, B, C, D\} \) and its associated LSA tree \( T_{LSA}(\mathcal{N}) \). Note that the reticulation edges (dashed) of \( \mathcal{N} \) have weight zero. The node \( v \) is the lowest stable ancestor of the reticulation node \( r_1 \) and we have to consider two paths when calculating the length of the edge \( e = (\text{lsa}(r_1), r_1) \): \( P_1 = (((v, u), (u, r_1)) \) with \( \text{length}(P_1) = 1 + 0 = 1 \) (recall that we have defined the lengths of reticulation edges to be zero) and \( P_2 = ((v, w), (w, r_1)) \) with length \( \text{length}(P_2) = 1 + 0 = 1 \). Thus, taking the average, we set \( \text{length}(\text{lsa}(r_1), r_1) = 1 \). Analogously, node \( \rho \) is the lowest stable ancestor of \( r_2 \) and we have to consider the paths \( P_3 = (((\rho, v), (v, w)), (w, r_2)) \) with \( \text{length}(P_3) = 1 + 1 + 0 = 2 \) and \( P_4 = ((\rho, x), (x, r_2)) \) with \( \text{length}(P_4) = 2 + 0 = 2 \). Thus, we set \( \text{length}(\text{lsa}(r_2), r_2) = 2 \). However, subsequently the edges \( (v, r_1) \) and \( (r_1, B) \) are merged into a new edge \( (v, B) \) of length \( 1 + 1 = 2 \) and analogously, the edges \( (\rho, r_2) \) and \( (r_2, C) \) are replaced by a new edge \( (\rho, C) \) of length \( 2 + 1 = 3 \) to finally yield the LSA tree associated with \( \mathcal{N} \). Note that \( T_{LSA}(\mathcal{N}) \) is not binary, because the root \( \rho \) has degree 3.

**Example 1.** Consider the phylogenetic tree \( T_1 \) on \( X = \{A, B, C, D\} \) depicted in Figure 1. Now consider the subset \( S = \{A, B\} \subseteq X \) of taxa. Then the phylogenetic diversity of \( S \) calculates as \( PD(S) = 2 + 1 + 1 + 1 = 5 \).

Based on phylogenetic diversity, we can now define the Shapley Value for phylogenetic trees. The Shapley Value for phylogenetic trees is used in different versions in the literature (cf. Wicke and Fischer (2017)), but we will use the so-called original Shapley Value throughout this paper.

**Definition 3 (Original Shapley Value).** Let \( T \) be a rooted phylogenetic tree with leaf set \( X \) and let \( PD(S) \) denote the phylogenetic diversity of \( S \subseteq X \). Then the Shapley Value for a taxon \( a \in X \) is defined as

\[
SV_T(a) = \frac{1}{n!} \sum_{S \subseteq X} (|S| - 1)! (n - |S|)! (PD(S) - PD(S \setminus \{a\}))
\]

where \( n = |X| \) and \( S \) denotes a subset of species containing taxon \( a \) (also sometimes referred to as ‘coalition’) and the sum runs over all such coalitions possible.

While the Shapley Value reflects the average contribution of a species to overall phylogenetic diversity and is thus a sensible prioritization criterion, its calculation is complicated. Therefore another index, the so-called Fair Proportion Index, has been introduced.

**Definition 4 (Fair Proportion Index).** For a rooted phylogenetic tree \( T \) with leaf set \( X \) the Fair Proportion Index of a taxon \( a \) is defined as

\[
FP_T(a) = \sum_e \frac{\lambda_e}{D_e}
\]

where \( \lambda_e \) is the length of edge \( e \).
where the sum runs over all edges $e$ on the path from $a$ to the root and $D_e$ denotes the number of leaves descendent from that edge.

The Fair Proportion Index can easily be calculated, but lacks a biological motivation. However, its use has been justified by its equivalence with the original Shapley Value.

**Theorem 1** (Fuchs and Jin (2015)). Let $T$ be a rooted phylogenetic tree with leaf set $X$. Then we have for all $a \in X$:

$$SV_T(a) = FP_T(a).$$

**Example 2.** Consider the phylogenetic tree $T_1$ on $X = \{A, B, C, D\}$ depicted in Figure 1. Here, we have $FP_{T_1}(A) = \frac{1}{3} + \frac{2}{7} = \frac{7}{21}$, $FP_{T_1}(B) = \frac{1}{3} + \frac{1}{2} + \frac{1}{7} = \frac{11}{21}$, $FP_{T_1}(C) = \frac{1}{3} + \frac{1}{2} + \frac{1}{7} = \frac{11}{21}$, and $FP_{T_1}(D) = \frac{2}{7} = 3$. Note that $FP_{T_1}(A) + FP_{T_1}(B) + FP_{T_1}(C) + FP_{T_1}(D) = 9$, which equals the total sum of all edge lengths in $T_1$. Also note that the Fair Proportion Indices of $T_1$ equal the Shapley Values of $T_1$.

### 3. Generalization of phylogenetic diversity

We are now in the position to present our approaches towards the generalization of phylogenetic diversity from trees to networks. We will introduce three approaches, one based on the calculation of spanning arborescences and subgraphs of a network, one based on the set of trees displayed by a network and one based on the LSA tree associated with a network.

#### 3.1. Phylogenetic (sub)net diversity

Recall that the phylogenetic diversity of a subset $S \subseteq X$ of taxa of a phylogenetic $X$-tree $T$ was calculated as the sum of branch lengths of the subtree of $T$ containing $S$ and the root. For a phylogenetic network $\mathcal{N}$ on $X$ and a subset $S \subseteq X$ of taxa, there may be more than one subtree, or to be precise, more than one arborescence (because a phylogenetic network is a directed graph) containing $S$ and the root. Thus, we suggest to consider an arborescence of minimum cost and introduce the so-called **phylogenetic net diversity**.

**Definition 5** (Phylogenetic net diversity). Let $\mathcal{N}$ be a rooted phylogenetic network on some taxon set $X$. For a subset $S \subseteq X$ of taxa we define the **phylogenetic net diversity** $PND(S)$ of $S$ as the sum of branch lengths in a minimum cost arborescence containing $S$ and the root.

Note that determining the minimum cost arborescence containing a subset $S \subseteq X$ of taxa and the root is formally an instance of the so-called directed Steiner tree problem or Steiner arborescence problem, which, in general, is an $NP$-hard problem (Karp (1972)).
Figure 3: Rooted binary phylogenetic network $N$ on $X = \{A, B, C, D\}$ and arborescences $A_1$ and $A_2$ containing $S = \{A, B\}$ and the root. The bold edges in $N$ depict the subgraph $N_{\{A, B\}}$ of $N$ containing $\rho$ and $S = \{A, B\}$. Note that all reticulation edges (dashed) have weight zero.

Example 3. Consider Figure 3, which depicts the rooted phylogenetic network $N$ on $X = \{A, B, C, D\}$ and the two arborescences $A_1$ and $A_2$ containing $S = \{A, B\}$ and the root. $A_1$ has weight $1 + 1 + 2 = 4$, while $A_2$ has weight $2 + 1 + 1 + 1 = 5$. Thus, $A_1$ is the minimum cost arborescence containing $S = \{A, B\}$ and the root and we retrieve the phylogenetic net diversity of $S = \{A, B\}$ as $PND(\{A, B\}) = 4$.

Example 4. Consider the rooted phylogenetic network $N$ on $X = \{A, B, C, D\}$ depicted in Figure 3 and set $S = \{A, B\}$. Then the subgraph $N_S$ of $N$ (highlighted with bold lines) has length $1 + 1 + 1 + 1 = 5$ and thus, $PSD(\{A, B\}) = 5$.

3.2. Embedded phylogenetic diversity

If species are subject to hybridization or horizontal gene transfer, their genome contains parts of the genome of both its ancestors. However, evolution at the nucleotide level rather than the genome level is still treelike, because a single nucleotide can always be traced back to one parent. Therefore, we suggest to consider the set of trees embedded in a network as an alternative approach towards the generalization of phylogenetic diversity from trees to networks.

Definition 7 (Embedded phylogenetic diversity). Let $N$ be a rooted phylogenetic network on some taxon set $X$. For a subset $S \subseteq X$ of taxa consider the subgraph $N_S$ of $N$ containing the root of $N$ and the taxa in $S$ (i.e., $N_S$ is the subgraph of $N$ containing all nodes and edges that lie on at least one path from the root of $N$ to any of the leaves in $S$). Then we define the phylogenetic subnet diversity $PSD(S)$ of $S$ as the sum of branch lengths in $N_S$.

Example 4. Consider the rooted phylogenetic network $N$ on $X = \{A, B, C, D\}$ depicted in Figure 3 and set $S = \{A, B\}$. Then the subgraph $N_S$ of $N$ (highlighted with bold lines) has length $1 + 1 + 1 + 1 + 1 = 5$ and thus, $PSD(\{A, B\}) = 5$.
embedded phylogenetic diversity of a subset $S \subseteq X$ of taxa, where $*$ is one of the following functions $\min, \max, \sum, \emptyset$ and define

$$PD_{T(N)}^{\min}(S) := \min_{T \in T(N)} \{PD_T(S)\},$$

(3)

$$PD_{T(N)}^{\max}(S) := \max_{T \in T(N)} \{PD_T(S)\},$$

(4)

$$PD_{T(N)}^{\sum}(S) := \sum_{T \in T(N)} PD_T(S),$$

(5)

$$PD_{T(N)}^{\emptyset}(S) := \frac{1}{|T(N)|} \sum_{T \in T(N)} PD_T(S),$$

(6)

where $|T(N)|$ is the number of phylogenetic $X$-trees displayed by $N$.

Note that $*$ can be replaced by other functions on the phylogenetic diversity of the trees in $T(N)$, but we will only consider the minimum, the maximum, the sum and the average value of phylogenetic diversity in the set of embedded trees as defined above.

Also note that we will only consider phylogenetic $X$-trees as elements of $T(N)$ and discard all other trees that may occur when decomposing the network into a set of trees (cf. Figure 1).

**Example 5.** Consider the rooted phylogenetic network $N$ on $X = \{A, B, C, D\}$ and its embedded trees $T_1, T_2$ and $T_3$ depicted in Figure 1. Now set $S = \{A, B\} \subseteq X$. Then we have $PD_{T_1}(S) = 5, PD_{T_2}(S) = 5$ and $PD_{T_3}(S) = 4$. Thus, we retrieve the different values of the embedded phylogenetic diversity of $S = \{A, B\}$ as $PD_{T(N)}^{\min}(S) = 4, PD_{T(N)}^{\max}(S) = 5, PD_{T(N)}^{\sum}(S) = 14$ and $PD_{T(N)}^{\emptyset}(S) = \frac{14}{3}$.

### 3.3. Relationship between the phylogenetic net diversity and the embedded phylogenetic diversity

Comparing the phylogenetic net diversity $PND$ and the minimum embedded phylogenetic diversity $PD_{T(N)}^{\min}$ for a subset $S \subseteq X$ of taxa, we see that they use a similar principle. While $PND(S)$ is defined as the weight of a minimum cost arborescence spanning $S$ and the root in a network $N$, $PD_{T(N)}^{\min}$ is defined as the weight of a minimum spanning tree/minimum cost arborescence spanning $S$ and the root in the set $T(N)$ of phylogenetic $X$-trees displayed by $N$. Thus, the two measures are related, but in general they are not identical. Consider, for example the rooted phylogenetic network $\mathcal{N}$ depicted in Figure 1 and set $S = \{A, B, C, D\}$. Then, we have $PD_{T(N)}^{\min}(S) = 9$, while $PND(S) = 8$.

However, we have the following relationship between $PND$ and $PD_{T(N)}^{\min}$:

**Proposition 1.** Let $\mathcal{N}$ be a binary rooted phylogenetic network on a taxon set $X$ with $k$ reticulation nodes and let $T(\mathcal{N})$ be the set of phylogenetic $X$-trees displayed by $\mathcal{N}$.
1. We have
\[ PND(S) \leq PD_{T(N)}^{\text{min}}(S) \] (7)
for all subsets \( S \subseteq X \) of taxa.

2. If \(|T(N)| = 2^k\), i.e. if all combinations of removing one reticulation edge for each reticulation node and suppressing nodes of both indegree 1 and outdegree 1 result in a phylogenetic \( X \)-tree, we have
\[ PND(S) = PD_{T(N)}^{\text{min}}(S). \] (8)

Remark. Note that \(|T(N)| = 2^k\) for example holds for so-called normal networks (cf. van Iersel et al. (2010)).

Proof of Proposition 1. Let \( N \) be a binary rooted phylogenetic network with root \( \rho \), taxon set \( X \) and \( k \) reticulation nodes. Let \( T(N) \) be the set of embedded trees and let \( R(N) = \{ r \mid r \text{ is a reticulation node of } N \} \) be the set of reticulation nodes of \( N \).

1. We show \( PD_{T(N)}^{\text{min}}(S) \geq PND(S) \).

For every \( T \in T(N) \) the phylogenetic diversity of a subset \( S \subseteq X \) of taxa is defined as the sum of branch lengths in the smallest arborescence spanning the taxa in \( S \) and the root. Clearly, the weight of any such arborescence cannot be smaller than the weight of a minimum cost arborescence spanning \( S \) and the root. In particular, we have
\[ \min_{T \in T(N)} \{ PD_T(S) \} = PD_{T(N)}^{\text{min}}(S) \geq PND(S). \]

2. Now, suppose that \(|T(N)| = 2^k\). We want to show that \( PND(S) = PD_{T(N)}^{\text{min}}(S) \). As we have \( PND(S) \leq PD_{T(N)}^{\text{min}}(S) \) (Equation (7)), it suffices to show \( PND(S) \geq PD_{T(N)}^{\text{min}}(S) \).

Let \( A_S \) be the minimum cost arborescence spanning \( S \) and the root in \( N \). By definition of an arborescence there is exactly one directed path from the root \( \rho \) to any other vertex \( v \in V(A_S) \). This implies that \( A_S \) contains at most one reticulation edge for each reticulation node \( r \in R(N) \), but never both reticulation edges directed into \( r \in R(N) \). If we now suppress nodes of both indegree 1 and outdegree 1 in \( A_S \) and add the weights of the edges which are merged into one edge by doing so, we retrieve a directed acyclic graph \( A'_S \), which contains the taxa in \( S \) and whose weight equals the weight of \( A_S \). By the construction of \( A'_S \), however, \( A'_S \) must be a sub-arborescence of some embedded tree \( T_{A_S} \in T(N) \), where the set of embedded trees is obtained by deleting one of the reticulation

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Formally, we have to re-establish the nodes of in- and outdegree 1 that were removed during the construction of \( T \in T(N) \) to make \( T \) a subgraph of \( N \). However, this does not affect the weights.
edges for each reticulation node and suppressing the resulting nodes of
indegree 1 and outdegree 1, and every combination of doing so results in
a phylogenetic \( X \)-tree (because we have assumed \( |T(N)| = 2^k \)). Thus, by
definition of \( PD \) for trees, the weight of \( A_S \) equals \( PD_{T_A_S}(S) \) and as \( T_{A_S} \)
is embedded in \( N \) we have

\[
PND(S) = PD_{T_A_S}(S) \geq \min_{T \in T(N)} \{ PD_T(S) \} = PD_{\min_{T(N)}}(S).
\]

Combining the above, we have \( PND(S) = PD_{\min_{T(N)}}(S) \) as claimed.

### 3.4. LSA associated phylogenetic diversity

As it can be difficult to determine the set of phylogenetic \( X \)-trees displayed
by a network \( N \) on \( X \), we now consider the LSA tree associated with a network. The LSA tree can be seen as a way to summarize the treelike content of a phylogenetic network, on which all its embedded trees agree, without explicitly having to consider these trees.

**Definition 8** (LSA associated phylogenetic diversity). Let \( N \) be a rooted phylogenetic network on some taxon set \( X \). Let \( S \subseteq X \) be a subset of taxa. Then we define the LSA associated phylogenetic diversity \( PD_{LSA}(S) \) as

\[
PD_{LSA}(S) := PD_{T_{LSA}(N)}(S),
\]

where \( PD_{T_{LSA}(N)}(S) \) is the phylogenetic diversity of \( S \) in the LSA tree \( T_{LSA}(N) \) associated with \( N \).

**Example 6.** Consider the rooted phylogenetic network \( N \) and its associated LSA tree \( T_{LSA}(N) \) depicted in Figure 2. Exemplarily, we set \( S = \{A,B\} \) and retrieve the LSA associated phylogenetic diversity of \( S \) as \( PD_{LSA}(S) = 2 + 2 + 1 = 5 \).

We have introduced a variety of ways to define the phylogenetic diversity of
a subset \( S \subseteq X \) of taxa in a network. However, the information about the phylogenetic diversity of a subset \( S \subseteq X \) of taxa in itself is not very useful for
taxon prioritization decisions. Thus, we now turn our attention towards the
generalization of phylogenetic diversity indices from trees to networks.

### 4. Generalization of phylogenetic diversity indices

After proposing different ways of generalizing the concept of phylogenetic
diversity from trees to networks, we will now turn our attention to the Fair
Proportion Index and the Shapley Value, two prioritization indices used in bio-
diversity conservation. Even though the Fair Proportion Index and the Shapley
Value are equivalent for rooted phylogenetic trees \( \) (Fuchs and Jin (2015)), they
differ significantly in their definition and computation. While the Fair Proportion
Index is directly based on a given rooted phylogenetic tree (cf. Definition
4), the definition of the Shapley Value is based on the phylogenetic diversity of subsets of taxa, and thus, only indirectly on a given phylogenetic tree (cf. Definition 3). To be precise, the calculation of the Shapley Value involves two steps:

1. Calculation of the phylogenetic diversity for all subsets of taxa based on a given phylogenetic tree.
2. Calculation of the Shapley Value for all taxa based on the phylogenetic diversity calculated in step 1.

This implies that we have two possibilities when extending the Shapley Value from trees to networks: We can either use any generalized definition of phylogenetic diversity (e.g. the phylogenetic net diversity, the embedded phylogenetic diversity or the LSA associated phylogenetic diversity) introduced above and calculate the Shapley Value based on this measure, or we can reduce the network to its treelike content (e.g. via the set of embedded trees or the LSA tree) and calculate the Shapley Value based on these trees. We will, however, start with the reduction of a network to its treelike content, which is also used to generalize the Fair Proportion Index to networks.

4.1. Embedded Shapley Value and Fair Proportion Index

Similar to the embedded phylogenetic diversity, we will now use the set $T(N)$ of phylogenetic $X$-trees displayed by a network $N$ on $X$ in order to define the so-called embedded Shapley Value and the embedded Fair Proportion Index.

**Definition 9** (Embedded Shapley Value, embedded Fair Proportion Index). Let $N$ be a rooted phylogenetic network on some taxon set $X$ and let $T(N)$ be the (multi)set of all rooted phylogenetic $X$-trees displayed by $N$. Then we use $DI_{T(N)}^*(a)$ with $DI \in \{SV, FP\}$ to denote the embedded Shapley Value or embedded Fair Proportion Index of a taxon $a \in X$, where $*$ stands for $\min, \max, \sum, \emptyset$ and define

\[
DI_{T(N)}^{\min}(a) := \min_{T \in T(N)} \{DI_T(a)\},
\]

\[
DI_{T(N)}^{\max}(a) := \max_{T \in T(N)} \{DI_T(a)\},
\]

\[
DI_{T(N)}^{\sum}(a) := \sum_{T \in T(N)} DI_T(a) \quad \text{and}
\]

\[
DI_{T(N)}^{\emptyset}(a) := \frac{1}{|T(N)|} \sum_{T \in T(N)} DI_T(a),
\]

where $|T(N)|$ is the number of phylogenetic $X$-trees displayed by $N$.

Note that as the Shapley Value and the Fair Proportion Index are equivalent on rooted phylogenetic trees [Fuchs and Jin (2015)], the embedded values coincide as well, i.e. $SV_{T(N)}^{\min}(a) = FP_{T(N)}^{\min}(a)$ for all $a \in X$ etc.
Example 7. Consider the rooted phylogenetic network $N$ on $X = \{A, B, C, D\}$ and its embedded trees $T_1, T_2$ and $T_3$ depicted in Figure 1 and fix taxon $A \in X$. Then we have $FP_{T_1}(A) = \frac{7}{3}$, $FP_{T_2}(A) = \frac{5}{2}$ and $FP_{T_3}(A) = \frac{11}{6}$. Thus, we retrieve the different versions of embedded Fair Proportion Index of $A$ as $FP_{\min T(N)}(A) = \frac{11}{6}$, $FP_{\max T(N)}(A) = \frac{5}{2}$, $FP_{\sum T(N)}(A) = \frac{20}{3}$ and $FP_{\emptyset T(N)}(A) = \frac{20}{9}$.

4.2. LSA associated Shapley Value and Fair Proportion Index

An alternative way of reducing a phylogenetic network to its treelike content is the LSA tree. Thus, we will now introduce the LSA associated Shapley Value and the LSA associated Fair Proportion Index.

Definition 10 (LSA associated Shapley Value, LSA associated Fair Proportion Index). Let $N$ be a rooted phylogenetic network on some taxon set $X$. Let $a \in X$ be a taxon in $X$. Then we use $DI_{LSA}(a)$ with $DI \in \{SV, FP\}$ to denote the LSA associated Shapley Value or LSA associated Fair Proportion Index and define

$$DI_{LSA}(a) := DI_{T_{LSA}(N)}(a),$$

where $DI_{T_{LSA}(N)}(a)$ is the respective diversity index (i.e. the Shapley Value or the Fair Proportion Index) in the LSA tree $T_{LSA}(N)$ associated with $N$.

Obviously, $SV_{LSA}(a) = FP_{LSA}(a)$ for all $a \in X$, because the two values coincide for rooted phylogenetic trees, thus they coincide in particular for the LSA tree.

Example 8. Consider the rooted phylogenetic network $N$ and its associated LSA tree $T_{LSA}(N)$ depicted in Figure 2 and fix taxon $a \in X$. Then the LSA associated Fair Proportion Index of $A$ is $FP_{LSA}(A) = \frac{1}{2} + \frac{2}{3} = \frac{5}{6}$.

4.3. Generalized Shapley Value

As the definition of the Shapley Value is only indirectly based on a given phylogenetic X-tree and just requires a measure of phylogenetic diversity for all subsets $S \subseteq X$ of taxa (cf. Definition 3), we now introduce an alternative way of calculating the Shapley Value for the taxa of a phylogenetic network $N$. We suggest to calculate the Shapley Value according to its definition and use any measure of generalized phylogenetic diversity (e.g. the phylogenetic net diversity, the embedded phylogenetic diversity or the LSA associated phylogenetic diversity) as an input. We call the resulting value the generalized original Shapley Value.

Definition 11 (Generalized Shapley Value). Let $N$ be a rooted phylogenetic network on some taxon set $X$ and let $T(N)$ be the (multi)set of all rooted phylogenetic X-trees displayed by $N$. Let $a \in X$ be a taxon in $X$ and let $PD(S)$ denote any generalized measure of phylogenetic diversity of a subset $S \subseteq X$ of taxa in $N$, i.e. $PD(S) \in \{PND(S), PSD(S), PD_{T(N)}^{\min}(S), PD_{T(N)}^{\max}(S), PD_{T(N)}^{\Sigma}(S)\}$,
Then we define the generalized original Shapley Value of \( a \) as

\[
SV_{PD}(a) = \frac{1}{n!} \sum_{S \subseteq X} \left( (|S| - 1)!((n - |S|)!\left(\mathcal{PD}(S) - \mathcal{PD}(S \setminus \{a\})\right) \right),
\]

where \( n = |X| \) and \( S \) denotes a subset of species containing taxon \( a \) and the sum runs over all such subsets possible.

Example 9. Consider the rooted phylogenetic network \( \mathcal{N} \) on \( X = \{A, B, C, D\} \) depicted in Figure 1. We now calculate the generalized original Shapley Value of taxon \( A \in X \) and choose the phylogenetic net diversity (cf. Definition \( 5 \)) as input. We have to consider the following subsets \( S \subseteq X: \{A\}, \{A, B\}, \{A, C\}, \{A, D\}, \{A, B, C\}, \{A, B, D\}, \{A, C, D\} \) and \( \{A, B, C, D\} \). Thus,

\[
SV_{PND}(A) = \frac{1}{4!} \sum_{S \subseteq X} \left( (|S| - 1)!(|X| - |S|)!((PND(S) - PND(S \setminus \{A\})) \right)
\]

\[
= \frac{1}{4!} \left[ (1 - 1)!((4 - 1)!3 - 0) + (2 - 1)!((4 - 2)!((4 - 3) + (5 - 3) + (6 - 3)) + (3 - 1)!((4 - 3)!((6 - 4) + (7 - 6) + (7 - 4)) + (4 - 1)!((4 - 4)!)(8 - 7) \right]
\]

\[
= \frac{1}{24} \left[ 1 \cdot 6 \cdot 3 + 1 \cdot 2 \cdot (1 + 2 + 3) + 2 \cdot 1 \cdot (2 + 1 + 3) + 6 \cdot 1 \cdot 1 \right]
\]

\[
= \frac{48}{24} = 2.
\]

4.4. Relationship between the different versions of the Shapley Value for phylogenetic networks

We now shortly compare the generalized Shapley Value and the embedded Shapley Value of a phylogenetic network \( \mathcal{N} \) on \( X \).

The first observation to make is that, in general,

\( SV_{PD_{\min}^T}(a) \neq SV_{\min}^T(a) \) and

\( SV_{PD_{\max}^T}(a) \neq SV_{\max}^T(a) \)

for \( a \in X \). Consider for example the rooted phylogenetic network \( \mathcal{N} \) on \( X = \{A, B, C, D\} \) depicted in Figure 1 and fix taxon \( A \). Then we have \( SV_{PD_{\min}^T}(A) = \frac{9}{4} \neq \frac{11}{6} = SV_{\min}^T(A) \) and \( SV_{PD_{\max}^T}(A) = \frac{13}{6} \neq \frac{5}{2} = SV_{\max}^T(A) \).

However, it is easy to see that for all \( a \in X \)
Proof. We only show (i), but (ii) follows analogously.

Recall that \( PD_{T(N)}(S) = \sum_{T \in T(N)} PD_T(S) \). Thus,

\[
SV_{PD_{T(N)}}(a) = SV_{T(N)}(a) = \sum_{S \subseteq X, a \in S} \left( \frac{(|S| - 1)!(n - |S|)!}{n!} \left( \sum_{T \in T(N)} PD_T(S) - \sum_{T \in T(N)} PD_T(S \setminus \{a\}) \right) \right) = \sum_{T \in T(N)} SV_T(a).
\]

On the other hand we have

\[
SV_{T(N)}(a) = \sum_{T \in T(N)} SV_T(a) = \sum_{T \in T(N)} \left( \frac{1}{n!} \sum_{S \subseteq X, a \in S} \left( (|S| - 1)!(n - |S|)! \left( \sum_{T \in T(N)} PD_T(S) - \sum_{T \in T(N)} PD_T(S \setminus \{a\}) \right) \right) \right) = \sum_{T \in T(N)} \left( (|S| - 1)!(n - |S|)! \left( \sum_{T \in T(N)} (PD_T(S) - PD_T(S \setminus \{a\})) \right) \right) \]

Thus,

\[
SV_{PD_{T(N)}}(a) = SV_{T(N)}(a).
\]

If we compare the LSA associated Shapley Value \( SV^{LSA} \) and the generalized Shapley Value \( SV_{PDLSA} \) that uses the LSA associated phylogenetic diversity as input, we see that all calculations are based upon the LSA tree associated with a network \( N \) on \( X \), thus for all \( a \in X \)

(iii) \( SV^{LSA}(a) = SV_{PDLSA}(a) \).

5. Software and Data

In order to calculate the different generalized measures of phylogenetic diversity and generalized diversity indices introduced above, we developed a software tool called NetDiversity, which is available from
The tool is written in the programming language Perl and uses modules from BioPerl (Stajich (2002)), in particular the Bio::PhyloNetwork package (Cardona et al. (2008a)). The program takes networks represented in the so-called extended Newick format (Cardona et al. (2008b)) as an input. Depending on the options chosen, the program either outputs any measure of generalized phylogenetic diversity for all subsets of taxa or any generalized diversity index for all taxa of the network.

We apply NetDiversity to a phylogenetic network of swordtails and platyfishes (*Xiphophorus*: Poeciliidae) (cf. Solís-Lemus and Ané (2016)). This is one of the few published hybridization networks, even though hybridization is suspected to have occurred in a variety of other organisms as well. The *Xiphophorus* hybridization network inferred in Solís-Lemus and Ané (2016) contains 24 species and 2 reticulation nodes (cf. Figure 4). Exemplarily, we use NetDiversity to calculate the different versions of the Fair Proportion Index for the *Xiphophorus* species. Note that there are $2^{24} = 16777216$ possible subsets of taxa for a network on 24 species, which is why we refrain from calculating any measure of generalized phylogenetic diversity for all subsets of *Xiphophorus* or the generalized Shapley value here. Table 1 summarizes the results. For the *Xiphophorus* network, the rankings obtained by the embedded Fair Proportion Indices and the LSA associated Fair Proportion Index are very similar. There are, however, two striking differences concerning the species *X. xiphidium* and *X. nezahuacoyotl*. While *X. xiphidium* is ranked low by $FP_{\text{min}}^{\text{T}(N)}$, it is placed among the top 10 species by all other indices. The other difference between the indices concerns *X. nezahuacoyotl*, a hybrid species. *X. nezahuacoyotl* is ranked first by $FP_{\text{LSA}}^{\text{T}(N)}$, while it is ranked 12th, 12th, and 15th by the other indices.

Thus, in case of the *Xiphophorus* network, the different versions of the generalized Fair Proportion Index yield similar results, but there are striking differences. In particular the question of whether hybrid species are of high or low importance for overall biodiversity remains to be considered from a biological perspective.

Figure 4: *Xiphophorus* hybridization network with 24 species and 2 reticulation nodes (see supporting information (S1 Text) for more information; Figure created with Dendroscope (Huson and Scornavacca (2012)).
Table 1: Embedded and LSA associated Fair Proportion Indices (rounded) for the *Xiphophorus* species. The numbers in brackets indicate how species are ranked by the different indices.

| Species          | $F_{P_{\min}}$ | $F_{P_{\max}}$ | $F_{P^\circ}$ | $F_{P^{LSA}}$ |
|------------------|----------------|----------------|---------------|--------------|
| *X. gordoni*     | 1.711 (1)      | 1.879 (3)      | 1.795 (3)     | 1.879 (4)    |
| *X. meyeri*      | 1.711 (1)      | 1.879 (3)      | 1.795 (3)     | 1.879 (4)    |
| *X. continens*   | 1.710 (3)      | 2.117 (1)      | 1.913 (1)     | 2.047 (2)    |
| *X. pygmaeus*    | 1.710 (3)      | 2.117 (1)      | 2.047 (2)     | 1.913 (1)    |
| *X. couchianus*  | 1.580 (5)      | 1.747 (7)      | 1.663 (5)     | 1.747 (8)    |
| *X. multilineatus* | 1.418 (6)    | 1.835 (5)      | 1.627 (6)     | 1.765 (6)    |
| *X. nigrensis*   | 1.418 (6)      | 1.835 (5)      | 1.627 (6)     | 1.765 (6)    |
| *X. birchmanni*  | 1.027 (8)      | 1.341 (9)      | 1.184 (8)     | 1.271 (10)   |
| *X. malinche*    | 1.027 (8)      | 1.341 (9)      | 1.184 (8)     | 1.271 (10)   |
| *X. monticolus*  | 0.796 (10)     | 0.796 (10)     | 0.796 (10)    | 0.796 (10)   |
| *X. clemenciae*  | 0.796 (10)     | 0.796 (10)     | 0.796 (10)    | 0.796 (10)   |
| *X. alvarezi*    | 0.782 (12)     | 0.782 (12)     | 0.782 (12)    | 0.782 (12)   |
| *X. mayae*       | 0.782 (12)     | 0.782 (12)     | 0.782 (12)    | 0.782 (12)   |
| *X. hellerii*    | 0.618 (14)     | 0.618 (14)     | 0.618 (14)    | 0.618 (14)   |
| *X. nezahuacoyotl* | **0.560 (15)** | **1.049 (12)** | **0.804 (12)** | **2.237 (1)** |
| *X. montezumae*  | 0.560 (15)     | 1.060 (11)     | 0.810 (11)    | 0.990 (12)   |
| *X. signum*      | 0.532 (17)     | 0.532 (20)     | 0.532 (19)    | 0.532 (20)   |
| *X. cortezi*     | 0.525 (18)     | 0.840 (13)     | 0.682 (17)    | 0.770 (17)   |
| *X. variatus*    | 0.450 (19)     | 0.576 (19)     | 0.494 (20)    | 0.578 (19)   |
| *X. ziphidiun*   | **0.305 (20)** | **1.717 (8)**  | **1.011 (10)** | **1.177 (9)** |
| *X. evelynae*    | 0.248 (21)     | 0.416 (21)     | 0.332 (21)    | 0.416 (21)   |
| *X. milleri*     | 0.147 (22)     | 0.285 (22)     | 0.216 (22)    | 0.285 (22)   |
| *X. andersi*     | 0.117 (23)     | 0.218 (23)     | 0.168 (23)    | 0.218 (23)   |
| *X. maculatus*   | 0.079 (24)     | 0.136 (24)     | 0.108 (24)    | 0.136 (24)   |
6. Discussion and Outlook

In this paper, we have introduced different approaches towards the generalization of phylogenetic diversity and phylogenetic diversity indices from trees to networks. Our approaches provide an extension to existing prioritization tools in conservation biology and allow for the consideration of phylogenetic networks in prioritization decisions. This is of importance if the evolutionary history of a set of species is known to be non-treelike, and thus cannot be represented by a phylogenetic tree. We have applied our methods to a phylogenetic network representing the evolutionary relationships among swordtails and platyfishes (*Xiphophorus*: Poeciliidae), whose evolution is characterized by widespread hybridization. We have seen that different biodiversity indices may induce striking differences in the ranking order of taxa for conservation. Therefore, we remark that further research concerning the biological plausibility of our approaches is necessary before they can be put into practice. This may be achieved when more phylogenetic networks for different groups of organisms become available and can be analyzed under both a biological and mathematical perspective. Decisions in biodiversity conservation and taxon prioritization do always require thorough examination and should include as much information as possible. Therefore we are currently working on the incorporation of inheritance probabilities into our approaches. For a reticulation node, e.g. a hybrid species, inheritance probabilities reflect the probability or relative frequency with which the hybrid species inherits its genetic material from each of its parents and thus provide additional information on the evolutionary history of species that can be taken into account in prioritization decisions.

Supporting Information

S1 Text. Supporting information file that contains the *Xiphophorus* hybridization network (Solís-Lemus and Ané [2016]), its LSA tree and its embedded trees.

Acknowledgements

We thank Volkmar Liebscher for helpful discussions on this research project. The first author also thanks the Ernst-Moritz-Arndt-University Greifswald for the Landesgraduiertenförderung studentship, under which this work was conducted.

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