Comparing the rankings obtained from two biodiversity indices: the Fair Proportion Index and the Shapley Value

Kristina Wicke · Mareike Fischer

Received: date / Accepted: date

Abstract The Shapley Value and the Fair Proportion Index of phylogenetic trees have been frequently discussed as prioritization tools in conservation biology. Both indices rank species according to their contribution to total phylogenetic diversity, allowing for a simple conservation criterion. While both indices have their specific advantages and drawbacks, it has recently been shown that both values are closely related. However, as different authors use different definitions of the Shapley Value, the specific degree of relatedness depends on the specific version of the Shapley Value – it ranges from a high correlation index to equality of the indices. In this note, we first give an overview of the different indices. Then we turn our attention to the mere ranking order provided by either of the indices. We show that even though the chance of two rankings being exactly identical (when obtained from different versions of the Shapley Value) decreases with an increasing number of taxa, the distance between the two rankings converges to zero, i.e. the rankings are becoming more and more alike. Moreover, we introduce our software package FairShapley, which was implemented in Perl and with which all calculations have been performed.

Keywords Phylogenetic diversity · Shapley Value · Fair Proportion Index · Ranking order · Ultrametric · Computation

1 Introduction

Due to limited financial means, biodiversity conservation programs often need to prioritize the species to conserve. Two indices used in this matter are the Shapley...
Value and the Fair Proportion Index. Both are based on phylogenetic trees and rank species according to their contribution to overall biodiversity.

The Shapley Value was first introduced by Haake et al. (2007) for unrooted trees and reflects the average biodiversity contribution of a species. The Fair Proportion Index, on the other hand, lacks a biological link to conservation, but is significantly easier to calculate and has been preferred in practice. Under a different name (ED for Evolutionary Distinctiveness) the Fair Proportion Index has for example been used in the ‘EDGE of Existence’ Project, established by the Zoological Society of London in 2007 (see Isaac et al. (2007)). However, Hartmann (2012) observed a strong correlation between the Shapley Value and the Fair Proportion Index on rooted trees, where the Shapley Value was calculated for the unrooted version of the tree by suppressing the root vertex. Very recently, Fuchs and Jin (2014) have extended the concept of the Shapley Value to rooted trees and have shown that the two indices are identical for these trees. They also introduced a slightly modified version of the Shapley Value, which again is highly correlated to the Fair Proportion Index.

In this note we first give an overview of the various versions of the Shapley Value and their respective relatedness with the Fair Proportion Index, before we focus on the mere ranking order of taxa obtained from different versions of the indices. Although the indices are highly correlated, they can result in different ranking orders, especially when the trees become large. We will show with a simulation study based on random trees that in fact, despite the increasing correlation as the number of species grows, different ranking orders are still more likely than equal ones. Therefore, in order to demonstrate what the correlation really implies, we treat the ranking lists as vectors and use both the so-called Manhattan distance and the Kendall tau distance to measure the difference between two rankings suggested by different indices. We then show that in both cases the distance between these rankings tends to 0 as the number of species grows.

All calculations in this manuscript were performed using our new software tool FairShapley, which has been made publicly available at http://www.mareikefischer.de/Software/FairShapley.pl. This tool, which was implemented in Perl, is able to calculate all versions of the Shapley Value as well as the Fair Proportion Index as explained in this paper.

2 Preliminaries

Before we can present our results, we need to introduce some notations and definitions. Recall that a phylogenetic tree is a connected, acyclic graph, where the leaves are bijectively labelled by some set \( X \) of species, which are also often called taxa. If such a tree has the additional property that all internal nodes have degree 3, it is called binary unrooted, and if all internal nodes have degree 3 except for one specified root node \( \rho \) of degree 2, the tree is called binary rooted. Throughout this paper, when we refer to trees, we always mean binary phylogenetic trees, and we always specify whether we are referring to rooted or unrooted ones. When we write \( T^u \), this notation refers to an unrooted binary phylogenetic tree, whereas \( T^r \) always refers to a rooted binary phylogenetic tree. In both cases, when we refer to the size of a tree, we mean the number \( n = |X| \) of taxa, i.e. the number of leaves of the tree under consideration. Note that a rooted tree can also be turned into
Comparing the rankings of two biodiversity indices

an unrooted tree by suppressing the root node \( \rho \), i.e. by deleting \( \rho \) and the two edges adjacent to it and re-connecting the two resulting degree-2 vertices with a new edge. We subsequently elaborate how turning a rooted tree into an unrooted one can change the various diversity indices.

In biodiversity conservation, the phylogenetic diversity of a set of species plays an important role. This concept captures how diverse or different a set of species is. Mathematically, this requires the trees under consideration to come with edge lengths (e.g. representing evolutionary time since the last common ancestor or substitution rates). Therefore, we assume all edges in the trees to have edge lengths assigned to them, and we denote the length of an edge \( e \) as \( \lambda_e \). Moreover, recall that a rooted tree is called ultrametric if the path lengths from all leaves to the root are identical. Here, the path lengths are calculated as the sum of all edge lengths on the path from a leaf to the root. The concept of ultrametric trees is also often referred to as molecular clock in biology.

We are now in the position to formally define phylogenetic diversity, or \( PD \) for short.

**Definition 1** The phylogenetic diversity (\( PD \)) of a binary phylogenetic tree is defined as follows:

1. For a rooted phylogenetic tree \( T_r \) with leaf set \( X \), the \( PD_r \) of a subset \( S \subseteq X \) of taxa is calculated by summing up the edge lengths of the phylogenetic subtree of \( T_r \) containing \( S \) and the root (i.e. the sum of branch lengths in the smallest spanning tree in \( T_r \) containing \( S \) and the root).
2. In case of an unrooted phylogenetic tree \( T_u \), the unrooted phylogenetic diversity, \( PD_u \), of a subset \( S \subseteq X \) of taxa is defined as the sum of edge lengths in the minimal spanning tree in \( T_u \) connecting those leaves. The \( PD \) of a single taxon is defined as 0.

Note that in an ultrametric tree, all taxa have the same \( PD_r \), and note that if you consider the unrooted version \( T_u \) of a rooted tree \( T_r \), the \( PD \) changes due to the different definitions. This is illustrated by the following example.

**Example 1** Consider Figure 1 which depicts trees \( T_r \) and \( T_u \) on taxon set \( X = \{A, B, C, D\} \). Note that here, \( T_u \) is the tree you get by suppressing the root of \( T_r \). Now consider the highlighted subset \( S = \{A, B\} \subseteq X \). The phylogenetic diversity of \( S \) can be calculated as follows: \( PD_r(S) = 1 + 1 + 1 + 1 = 4 \), and \( PD_u(S) = 1 + 1 = 2 \). The difference between the two definitions of diversity can be explained by the path of length 2 connecting \( S \) with the root, which is disregarded in the unrooted case.

One more concept we need before we can turn our attention to diversity prioritization indices is the concept of a ranking. Here, a ranking \( r \) is just an ordered list with \( n = |X| \) entries which contains all elements of \( X \). Let \( x, y \in X \). We say that a function \( f : X \rightarrow \mathbb{R} \) induces the ranking \( r_f \), if the position of \( x \) in \( r_f \) is smaller than the position of \( y \) precisely if \( f(x) \geq f(y) \). So a ranking simply orders the elements of \( X \) in decreasing order according to the function \( f \) under consideration.

**Example 2** Let \( X = \{A, B, C, D\} \). Let \( f(A) = 0.5, f(B) = 3, f(C) = 0.2 \) and \( f(D) = 1.5 \). Then the induced ranking \( r_f \) is: \( B, D, A, C \).
Last but not least, recall that the so-called Manhattan distance \( d_1 \) (also known as \( L_1 \) distance or \( l_1 \) metric) between two vectors \( r, s \in \mathbb{R} \) is defined as follows:

\[
d_1(r, s) = \|r - s\| = \sum_{i=1}^{n} |r_i - s_i|,
\]

while the so-called Kendall tau distance counts the number of pairwise disagreements between two rankings:

\[
d_\tau(r, s) = |\{(i, j) : i < j, (r(i) < r(j) \land s(i) > s(j)) \lor (r(i) > r(j) \land s(i) < s(j))\}|.
\]

We will later on use these metrics to measure the difference between two rankings.

Now we are in a position to introduce the biodiversity indices, which we will analyze in the following.

2.1 Various indices for biodiversity conservation

In this section, we will present and analyse some indices for biodiversity conservation, which have recently been discussed in the literature. All of these indices turn out to be related, but as different authors use different definitions of these indices, their results sometimes differ. We will therefore give an overview about the relationships of the various definitions.

The first index we want to introduce is the Fair Proportion Index, which is only defined for rooted trees.

**Definition 2 (Fair Proportion Index)** For a rooted phylogenetic tree \( T_r \) with leaf set \( X \) the Fair Proportion Index of a taxon \( a \) is defined as

\[
FPT_r(a) = \sum_{e} \frac{\lambda_e}{D_e},
\]

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.

It can be easily shown that the sum of all fair proportion indices for a given species set \( X \) equals the total branch length of the given tree.

**Example 3** In Figure 1, \( FPT_r(A) = \frac{1}{4} + \frac{1}{2} + \frac{1}{4} = \frac{4}{9} \), \( FPT_r(B) = \frac{1}{4} + \frac{1}{2} + \frac{1}{3} = \frac{11}{16} \), \( FPT_r(C) = \frac{1}{4} + \frac{1}{2} = \frac{3}{4} \) and \( FPT_r(D) = \frac{1}{4} = 3 \). Altogether, we have \( FPT_r(A) + FPT_r(B) + FPT_r(C) + FPT_r(D) = 9 \), which equals the total sum of all branch lengths in \( T_r \). Moreover, the ranking induced by the Fair Proportion Index in this case is \( (D, B, A, C) = (D, B, A, C) \).

As has been shown in the previous example, the Fair Proportion Index can easily be calculated. However, it does not have a direct biological justification. Therefore, another index from evolutionary game theory was proposed and adjusted to phylogenetic conservation, namely the so-called Shapley Value [Haake et al. (2007); Hartmann (2012); Fuchs and Jin (2014)]. However, as various authors use slightly different versions of this index, we present three different definitions here, the first of which we call the original Shapley Value, which can be defined both for rooted and unrooted trees.
Definition 3 (Original Shapley Value) Let $T^r$ be a rooted phylogenetic tree with leaf set $X$ and let $PD^r(S)$ denote the phylogenetic diversity of $S \subseteq X$. Then the Shapley Value for a taxon $a \in X$ is defined as

$$SV_{T^r}(a) = \frac{1}{n!} \sum_{S \subseteq X, a \in S} (|S| - 1)!(|n - |S|)!((PD^r(S) - PD^r(S \setminus \{a\})),$$  \hspace{1cm} (2)

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. Similarly, for an unrooted tree $T^u$ with leaf set $X$ we have

$$SV_{T^u}(a) = \frac{1}{n!} \sum_{S \subseteq X, a \in S} (|S| - 1)!(|n - |S|)!((PD^u(S) - PD^u(S \setminus \{a\}))).$$  \hspace{1cm} (3)

Note that the definition of the original Shapley Value is basically the same for rooted and unrooted trees. The only difference is how the phylogenetic diversity of subsets is defined (i.e. $PD^r$ vs. $PD^u$). For rooted trees, however, this value coincides with the Fair Proportion Index, i.e. $SV_{T^r} = FP_{T^r}$, which was recently shown by Fuchs and Jin (2014).

We now present an example for the original Shapley Value.

Example 4 We calculate $SV_{T^r}(A)$ for the tree depicted in Figure 1 (a). Note that the possible subsets $S \subseteq X = \{A, B, C, D\}$ which contain $A$ are: $\{A\}$, $\{A, B\}$, $\{A, C\}$, $\{A, D\}$, $\{A, B, C\}$, $\{A, B, D\}$, $\{A, C, D\}$ and $\{A, B, C, D\}$. Thus, we have to consider 8 summands when calculating $SV_{T^r}(A)$:

$$SV_{T^r}(A) = \frac{1}{4!} \sum_{S, A \in S} (|S| - 1)!(|X| - |S|)!((PD^r(S) - PD^r(S \setminus \{A\}))$$

$$= \frac{1}{4!} \left[ (1 - 1)!(4 - 1)!(3 - 0) + (2 - 1)!(4 - 2)!(4 - 3) + (5 - 3) + (6 - 3))$$

$$+ (3 - 1)!(4 - 3)!(6 - 5) + (7 - 6) + (8 - 6))$$

$$+ (4 - 1)!(4 - 4)!(9 - 8) \right]$$

$$= \frac{11}{6}$$

Note that, as implied by the results of Fuchs and Jin (2014), this value coincides with $FP^r(A)$ as calculated above, but the calculation is much more involved. Moreover, a similar calculation yields $SV_{T^u}(A) = \frac{19}{12}$, which shows that the original Shapley Value for the rooted and unrooted versions of the tree depicted by Figure 1 differ due to the different underlying definitions of phylogenetic diversity.

Additionally to the original Shapley Value, Fuchs and Jin (2014) also introduced a modified version of the Shapley Value, which we will call modified Shapley Value and which we denote by $\tilde{SV}$ in the following. The difference between the original and the modified versions of the Shapley Value is that the first considers all subsets of taxa which contain a certain taxon, whereas the latter only considers subsets of size at least 2 (i.e. $|S| \geq 2$).
Definition 4 (Modified Shapley Value) Let $T^r$ be a rooted and $T^u$ be an unrooted phylogenetic tree with leaf set $X$ and let $PD^r(S)$ and accordingly $PD^u(S)$ denote the phylogenetic diversity of a subset $S \subseteq X$. Then the modified Shapley Value for a taxon $a$ is defined as

\[
\tilde{SV}^r_{T^r}(a) = \frac{1}{n!} \sum_{S:a \in S \atop |S| \geq 2} (|S| - 1)! (n - |S|)! (PD^r(S) - PD^r(S \setminus \{a\}))
\]  

(4)

in the rooted case and

\[
\tilde{SV}^u_{T^u}(a) = \frac{1}{n!} \sum_{S:a \in S \atop |S| \geq 2} (|S| - 1)! (n - |S|)! (PD^u(S) - PD^u(S \setminus \{a\}))
\]  

(5)

in the unrooted case, where $n = |X|$ and the sum runs over all coalitions $S$ containing taxon $a$ and at least one other taxon.

Comparing the original and the modified Shapley Value, it can be easily shown that

\[
SV^r_{T^r}(a) = \tilde{SV}^r_{T^r}(a) + \frac{PD^r(a)}{n} \quad \text{and} \quad SV^u_{T^u}(a) = \tilde{SV}^u_{T^u}(a) + \frac{PD^u(a)}{n} = \tilde{SV}^r_{T^r}(a).
\]  

(6)

(7)

Here, the last equality follows from the fact that $PD^u(S) = 0$ whenever a set $S \subseteq X$ contains only one taxon.

Hartmann (2012) states a correlation result for the Fair Proportion Index and the Shapley Value, but does not go into the details of the definition of the Shapley Value that he uses. Fuchs and Jin (2014) suggest that the modified Shapley Value was used in Hartmann (2012). We think, however, that Hartmann (2012) used yet another version of the Shapley Value, namely the original Shapley Value of the unrooted tree derived from the original tree by suppressing the root node. The reason why we think so is that, while Hartmann (2012) does not give a definition of phylogenetic diversity, he does state a definition of the Shapley Value, and the sum there ranges over all subsets containing a certain taxon, not only subsets of size at least 2. But he cannot be using the original Shapley Value for rooted trees, because otherwise his results would have led to equality of the Shapley Value and the Fair Proportion Index rather than only a strong correlation.

So this leads to yet another version of the Shapley Value, which we will call the unrooted Shapley Value on rooted trees, or unrooted rooted Shapley Value for short, and which we denote by $\tilde{SV}^r_{T^r}$.

Definition 5 For a rooted phylogenetic tree $T^r$ with leaf set $X$ we retrieve the unrooted Shapley Value on rooted trees of a taxon $a$ as

\[
\tilde{SV}^r_{T^r}(a) = SV^u_{T^r}(a),
\]  

(8)

where $SV^u_{T^r}(a)$ is the original Shapley Value of $a$ in the corresponding unrooted tree $T^u$. 
Recall that turning a rooted tree $T^r$ into an unrooted tree $T^u$ causes a change in the definition of phylogenetic diversity (i.e. a shift from $PD^r$ to $PD^u$). Thus, the unrooted Shapley Value on a rooted tree does not necessarily coincide with the original Shapley Value on the rooted tree. The two indices are, however, highly correlated (see Hartmann (2012)). However, note that this analysis is somewhat counterintuitive as the Fair Proportion Index is only defined for rooted trees, and in Hartmann (2012), only rooted trees are depicted, but for the Shapley Value still the unrooted version of the rooted tree seems to be used.

Anyway, just as the unrooted Shapley Value on a rooted tree need not coincide with the original Shapley Value on the rooted tree, it does not necessarily agree with the modified Shapley Value on the rooted tree, but again, the indices are closely related.

Summarizing the above, we have:

- $SV_{T^r} = FP_{T^r}$,
- $SV_{T^r} \neq SV_{T^u}$, but $SV_{T^r}(a) = \tilde{SV}_{T^r}(a) + \frac{PD^r(a)}{n}$ for all $a \in X$,
- $SV_{T^r} \neq \tilde{SV}_{T^r}$, but there is a high correlation between the two values (Hartmann (2012)),
- $SV_{T^u} = \tilde{SV}_{T^r}$, where $T^u$ denotes the unrooted version of $T^r$.

We finish this section with a few more examples.

**Example 5** Consider again Figure 1. As mentioned above, we have $FP_{T^r}(A) = SV_{T^r}(A) = \frac{11}{6}$. Moreover, we have $SV_{T^r}(A) = \frac{13}{12}$. For $T^u$ we have $SV_{T^u}(A) = \frac{19}{12}$. Note that $SV_{T^r}(A) \neq SV_{T^u}(A) \neq SV_{T^u}(A) = \tilde{SV}_{T^r}(A)$.

![Figure 1](image_url)

(a) Rooted tree $T^r$ with leaf set $\{A, B, C, D\}$.
(b) Unrooted tree $T^u$, which is derived from $T^r$ by suppressing the root node.

### 3 Comparing the rankings induced by the different indices

Both the original and modified Shapley Value and the unrooted Shapley Value on rooted trees and the original Shapley Value are highly correlated, which was shown in Fuchs and Jin (2014) and Hartmann (2012), respectively. But even if the
correlation index goes to 1 as the number of taxa goes to infinity, the indices can still result in different ranking orders of the taxa.

In the following we will first compare the rankings obtained from the original and modified Shapley Value and afterwards the rankings obtained from the original and unrooted Shapley Value on rooted trees.

For each analysis we have generated some random trees (the details of which will be explained in the subsequent sections). We then calculated the rankings obtained from the different versions of the Shapley Value and counted the number of cases, where the rankings were identical. Up until this step we allowed the rankings to include ties, i.e. two or more taxa could share the same position in the ranking, when their Shapley Values were identical. However, for ease of computation in the subsequent analyses we turned the rankings into permutations by dissolving ties arbitrarily.

Therefore, we first translated the rankings into vectors of length \( n = |X| \) as follows: Let \( r_1, r_2 \) be two rankings. We pick one of them, say \( r_1 \), as the reference, and associate with \( r_1 \) the ranking vector \( v_{r_1} = (1, 2, \ldots, n) \). Then, we consider \( r_2 \) and build the ranking vector \( v_{r_2} \) as follows. If the \( j^{th} \) element of \( r_2 \) occurs at the \( j^{th} \) position in \( r_1 \), then the \( i^{th} \) element of \( v_{r_2} \) contains number \( j \).

**Example 6** Suppose \( X = \{A, B, C, D\} \), and suppose that you have obtained two rankings \( r_1 = (A, C, D, B) \) and \( r_2 = (C, D, A, B) \) from two different prioritization indices. Then, picking \( r_1 \) as the reference, you get vector \( v_{r_1} = (1, 2, 3, 4) \) and vector \( v_{r_2} = (2, 3, 1, 4) \).

Note that the vectors associated with the rankings are permutations of the numbers 1, \ldots, \( n \). These vectors now allow us to calculate their Manhattan distance \( d_1(v_{r_1}, v_{r_2}) \) and Kendall tau distance \( d_\tau(v_{r_1}, v_{r_2}) \). However, since we want to observe the behaviour of the different prioritization indices for increasing numbers of taxa, we need to normalize the calculated distances. This is due to the fact that whenever the number of taxa increases, even small differences between two rankings have a higher impact on the distance. For example, if you compare the rankings (1, 2) and (2, 1), their Manhattan distance is \( d_1 = 1 + 1 = 2 \), and it is maximal in the sense that the two rankings could not be any more different. However, the Manhattan distance of the rankings (1, 2, 3, 4, 5) and (1, 2, 5, 4, 3) is \( d_1 = 0 + 0 + 2 + 0 + 2 = 4 \), and thus higher than the distance between the two rankings mentioned first, even though here only two out of five taxa swapped their places in the ranking. So we need to normalize in order to take into account that whenever the number of taxa increases, the maximum possible Manhattan distance increases, too. So we divide exactly by this factor.

Thus, we define the normalized Manhattan distance \( d'_1(r_1, r_2) \) for two rankings \( r_1 \) and \( r_2 \) with associated ranking vectors \( v_{r_1} \) and \( v_{r_2} \) as follows:

\[
d'_1(r_1, r_2) = \frac{d_1(v_{r_1}, v_{r_2})}{\max_{r', s'} d_1(v_{r'}, v_{s'})}.
\]

Note that the maximum in the denominator is obtained when \( r' = (1, 2 \ldots, n) \) and \( s' = (n, n-1, \ldots, 1) \).

Accordingly, we normalize the Kendall tau distance by the maximal number of pairwise disagreements that can occur between two rankings. One can easily see that this number equals \( \frac{n(n-1)}{2} \) (where \( n \) is the length of the ranking) and
Comparing the rankings of two biodiversity indices

again is obtained when one ranking is the reverse of the other. Thus, we define the normalized Kendall tau distance as follows:

\[ d^*_\tau(r_1, r_2) = \frac{d_\tau(r_1, r_2)}{n(n-1)/2}, \quad \text{where } n = |r_1| = |r_2|. \]

Example 7 Consider the rooted tree \( T^r \) depicted in Figure 2 and the different versions of the Shapley Value for its taxa as listed in the corresponding table.

By breaking ties arbitrarily we obtain the rankings \( r = (A, C, B, D), s = (A, C, D, B) \) and \( t = (D, A, C, B) \) from \( SV, \tilde{SV} \) and \( \hat{SV} \), respectively. Using \( r \) as the reference vector, we obtain \( v_r = (1, 2, 3, 4), v_s = (1, 2, 4, 3) \) and \( v_t = (4, 1, 2, 3) \). The maximal Manhattan distance between two vectors \( r', s' \) of length 4, containing the elements \( \{1, 2, 3, 4\} \) is \( d_1(r', s') = 8 \) and the maximal Kendall tau distance is \( d_2(r', s') = 6 \). Thus, we have \( d_1^*(r, s) = \frac{2}{8}, d_1^*(r, t) = \frac{6}{8}, d_2^*(r, s) = \frac{1}{6} \) and \( d_2^*(r, t) = \frac{3}{6} \).

We are now in a position to compare the different versions of the Shapley Value.

3.1 Original vs. modified Shapley Value

We now compare the ranking order of taxa obtained from the original and the modified Shapley Value. Recall that \( SV_{T^r}(a) \) and \( \tilde{SV}_{T^r}(a) \) differ only by the summand \( \frac{PD^*(a)}{n} \) (see Equation [8]). Therefore, note that the difference between the
two versions of the Shapley Value can be of any size. In particular, if we choose the branch lengths of $T^r$ so long that $PD^r(a) \geq n$ for all $a \in X$, the difference between $SV^r_T(a)$ and $\tilde{SV}^r_T(a)$ will increase as $n$ increases. But on the other hand, it can easily be seen that the values are highly correlated, because if $\tilde{SV}^r_T(a)$ gets larger, so does $SV^r_T(a)$ (by Equation (6)). So the values can be made arbitrarily different, but the correlation necessarily affects the ranking of the different taxa. This motivates our analysis of the rankings obtained from the two values instead of the values themselves. We will see in our simulation study that the rankings grow more and more alike with an increasing tree size.

However, before we present our simulation result, we state the following simple lemma which makes such a simulation unnecessary for ultrametric trees.

**Proposition 1** Let $T^r$ be a rooted binary phylogenetic tree on taxon set $X$. If $T^r$ is ultrametric, then the rankings implied by $SV^r_T(a)$ and $\tilde{SV}^r_T(a)$ are identical.

**Proof** In ultrametric trees, all paths from the root to a leaf are of the same length, say $k$. This implies $PD(a_1) = \ldots = PD(a_n) = k$ for all leaves $a_1, \ldots, a_n$. Using Equation (6), this leads to $SV^r_T(a) = \tilde{SV}^r_T(a) + \frac{k}{n}$ for all $a \in X$. Thus, the original and the modified Shapley Values still differ in ultrametric trees, but the difference is the same for all taxa and therefore the ranking order obtained from either of the two indices will be the same.

So for ultrametric trees, Proposition 1 shows equality between the rankings. Therefore, our subsequent analysis is only concerned with non-ultrametric trees. In particular, we want to find out how quickly (relative to the number $n$ of taxa) the rankings of the two indices $SV^r_T(a)$ and $\tilde{SV}^r_T(a)$ on average coincide for increasing $n$.

For this analysis, we used R [R Development Core Team (2014)] to generate two sets of 100 random trees, respectively, for each $n$. We ran the analysis for $n = 10, 20, \ldots, 100$. For each $n$, the first tree set consists of randomly chosen tree topologies, where we assumed a uniform distribution of all possible rooted binary tree topologies on $n$ taxa. After randomly picking a tree topology, we assigned random edge lengths uniformly from the interval $[1, 10]$.

For the second set, we chose a more common way to generate trees with branch lengths. For each $n$, the second set consisted of 100 random trees which were generated under a birth-death model with birth rate $\mu = 1$ and death rate $\nu = 1$. Please note that even when a birth-death model is considered, it does not make much sense to consider some of the lineages as extinct, as biodiversity conservation can only aim at present-day species. So in this case, the birth-death model is only used to simulate a suitable tree shape, but not to represent the evolutionary history of the $n$ species under investigation. We always consider all $n$ lineages as extant, and the branch lengths are some measure of difference between the species.

After generating the two sets of 100 random trees for each $n$, we calculated $SV^r_T(a)$ and $\tilde{SV}^r_T(a)$ for all $a \in X$. Then we inferred the induced rankings of $SV^r_T$ and $\tilde{SV}^r_T$ and calculated both the normalized Manhattan distance and the normalized Kendall tau distance between the two rankings. These values were then summarized in the boxplots depicted in Figure 3 and Figure 4 respectively (all Figures were generated using MATLAB (2013)). On the $x$ axis, we denoted both the number $n$ of taxa as well as the absolute counts (in brackets) of rankings which were identical.
For both sets of trees, the number of identical rankings decreases from 16 or 20, respectively, for 10 taxa down to 0 for 30 or more taxa. Thus, the rankings obtained from the two versions of the Shapley Value tend to differ when the tree becomes large despite the high correlation.

However, the amount of dissimilarity between the rankings decreases with an increasing tree size, as both the variability of the obtained distances within a tree set of fixed size (as depicted by the boxplots in Figure 3 and Figure 4) and the mean distance (see Figures 3 and 4) decrease with a growing number of taxa.

Note that the overall tendency is both captured by the Manhattan distance and the Kendall tau distance, even though they are two different concepts: The Manhattan distance is a metric measuring the difference between arbitrary vectors (not only rankings), whereas the Kendall tau distance is explicitly aiming at rankings.

In summary we can say that the original and modified Shapley Value are more likely to result in an identical ranking order for small trees than for large trees. However, when they do not result in exactly the same ranking, the rankings are on average ‘more similar’ for large trees than for small trees (in terms of the both the normalized Manhattan and Kendall tau distance).

3.2 Original Shapley Value vs. unrooted rooted Shapley Value

We now compare the Original Shapley Value and the unrooted rooted Shapley Value. In this case, we have to consider both ultrametric and non-ultrametric trees, because in both cases the ranking order may differ. In the non-ultrametric case we used the set of birth-death trees from above (see Section 5.1) for the analysis, while we generated a set of random trees under a Yule-model (i.e. a pure birth process) for the ultrametric case.

Again, we counted the number of identical rankings and calculated the normalized Manhattan and Kendall tau distances (see Figure 4 and Figure 5, respectively).

We first notice that the number of cases where the rankings obtained from the original and unrooted rooted Shapley Value are identical is higher for Yule trees (ultrametric) than for birth-death trees (non-ultrametric). Similarly, the variability of both the normalized Manhattan distance and the normalized Kendall tau distance itself, is smaller in Yule trees than in birth-death trees. Still, in both cases it decreases with an increasing number of taxa. Notice, however, the difference in the scaling of the y-axis for Yule trees and birth-death trees. In all cases, both the mean normalized Manhattan and Kendall tau distances between rankings obtained from the original Shapley Value and rankings obtained from the unrooted rooted Shapley Value are approximately ten times smaller in Yule trees than in birth-death trees.

In summary we can say that the number of times where we obtain identical rankings from the two versions of the Shapley Value decreases with a growing number of taxa. At the same time, the normalized distances (either Manhattan or Kendall tau) between the rankings decrease. Thus, in those cases where the rankings are not exactly identical, they tend to be ‘more similar’ for large trees than for small trees (again in terms of the normalized Manhattan and Kendall Tau
Fig. 3: Boxplots and plot of the mean of the normalized Manhattan distance between rankings obtained from the modified and the original Shapley Value for 100 trees of size \( n = 10, 20, \ldots, 100 \), respectively. The numbers in round brackets in the boxplots denote the number of identical rankings, e.g. in case of the birth-death trees with 10 taxa, we counted 20 identical and 80 dissimilar rankings.
Comparing the rankings of two biodiversity indices

Fig. 4: Boxplots and plot of the mean of the normalized Kendall tau distance between rankings obtained from the modified and the original Shapley Value for 100 trees of size $n = 10, 20, \ldots, 100$, respectively. The numbers in round brackets in the boxplots denote the number of identical rankings, e.g. in case of the birth-death trees with 10 taxa, we counted 20 identical and 80 dissimilar rankings.
This reflects the effect which we have already observed for the rankings obtained from the modified and the original Shapley Value (see Section 3.1). However, the impact of using the unrooted rooted Shapley Value as opposed to the original Shapley Value is higher for non-ultrametric trees than for ultrametric trees. The two indices can result in different rankings in both cases, but they are less different in the ultrametric case. Remember that the original and modified Shapley Value always lead to the same ranking order of taxa for ultrametric trees, which the original and unrooted rooted Shapley Value may not do. Still, ultrametricity seems to imply that it is less important which version of the Shapley Value we use to obtain a ranking of taxa.

4 Software

In order to calculate the different versions of the Shapley Value, we developed a program called FairShapley, which is available from http://www.mareikefischer.de/Software/FairShapley.pl. A readme file containing a short manual is available at http://www.mareikefischer.de/Software/FairShapleyREADEME.txt. The tool is written in the programming language Perl and uses modules from BioPerl (Stajich (2002)). In contrast to existing tools for the Fair Proportion Index and the Shapley Value (Vos et al (2011)), which use the unrooted version of the Shapley Value (regardless of the tree being rooted or not) and arbitrarily root unrooted trees in case of the Fair Proportion Index, our program explicitly distinguishes between rooted and unrooted trees. It allows for the computation of both the original Shapley Value (which coincides the Fair Proportion Index if the tree is rooted, as we pointed out earlier), the modified Shapley Value and the unrooted Shapley Value on rooted trees. The program takes trees represented in the so-called Newick format (cf. Felsenstein et al (2000)) as an input. This format uses brackets, and two closely related species are grouped closely together. Moreover, a binary tree has two entries at each bracket level – expect for unrooted trees, which have three entries at the uppermost level. For example, the trees in Figure 1 can be denoted by $T^r = (((A : 1, B : 1), C : 2) : 1, D : 3)$ and $T^u = ((A : 1, B : 1) : 1, C : 2, D : 4)$. Note that the numbers denote the edge lengths, e.g. $A : 1$ means that the edge leading to leaf $A$ has length 1. The program outputs the ranking order of taxa obtained from any version of the Shapley Value.

5 Discussion

In this paper, we summarized the different versions of the Shapley Value which can be found in the literature and which have different relationships with one another as well as with the frequently used Fair Proportion Index. We also showed that even though the different definitions are all highly correlated, the rankings they induce are hardly ever identical when the number $n$ of taxa under investigation is large. But the difference between the different rankings converges to zero as $n$ grows. We could show that these findings are true for two different types of metrics: the Manhattan distance, which is defined for general vectors, as well as for the Kendall tau distance, which is aiming at rankings. However, for the Kendall tau distance, ties can be problematic: It is unclear how to compare rankings, that are, say,
Comparing the rankings of two biodiversity indices

Fig. 5: Boxplots and plot of the mean of the normalized Manhattan distance between rankings obtained from the original Shapley Value and the unrooted Shapley Value on rooted trees for 100 trees of size $n = 10, 20, \ldots, 100$, respectively. The numbers in round brackets in the boxplots denote the number of identical rankings, e.g. in case of the birth-death trees with 10 taxa, we counted 3 identical and 97 dissimilar rankings.
Fig. 6: Boxplots and plot of the mean of the normalized Manhattan distance between rankings obtained from the original Shapley Value and the unrooted Shapley Value on rooted trees for 100 trees of size $n = 10, 20, \ldots, 100$, respectively. The numbers in round brackets in the boxplots denote the number of identical rankings, e.g. in case of the birth-death trees with 10 taxa, we counted 3 identical and 97 dissimilar rankings.
(1, 2, 2, 3) and (1, 2, 3, 3), which is why Kendall tau only works for rankings which use all numbers from 1 to $n$ exactly once. This led to the necessity of breaking ties arbitrarily in order to use Kendall tau. But note that breaking ties arbitrarily can lead to a situation where two rankings that used to be identical (i.e. they contained the same ties), now produce a distance greater than zero, because their ties were dissolved in different ways.

**Example 8** Suppose $X = \{A, B, C, D\}$, and suppose that you have obtained two rankings $r_1 = (A, C, D, B)$ and $r_2 = (A, C, D, B)$. By translating both rankings individually and allowing them to include ties, we see that $v_{r_1} = (1, 2, 2, 4) = v_{r_2}$, thus $r_1$ and $r_2$ are identical. However, breaking ties arbitrarily can lead to $r_1' = (A, C, D, B)$ and $r_2' = (A, D, C, B)$. If we now use $r_1'$ as the reference, we obtain $v_{r_1'} = (1, 2, 3, 4)$ and $v_{r_2'} = (1, 3, 2, 4)$ and thus, $d_τ^1(r_1, r_2) = \frac{1}{3} > 0$.

Similarly, suppose you have obtained $r_3 = (A, D, C, B)$. Then $r_1$ and $r_3$ are not identical (because $r_1$ contains a tie and $r_3$ does not), but the distance between $r_1$ and $r_3$ can be either zero (if $r_1$ is dissolved as $(A, D, C, B)$) or greater than zero (if $r_1$ is dissolved as $(A, C, D, B)$).

The Manhattan distance theoretically does not suffer from this problem – in fact, all vectors can be compared, not just those induced by a permutation. But ties cause another problem for the Manhattan distance: When we for example have rankings $r_1$ and $r_2$ on species $A$, $B$ and $C$, such that in $r_1$ all three species are on the first rank because they had the same value assigned, i.e. $r_1 = (1, 1, 1)$, then if the second ranking implies that $A$ has a higher value assigned than both $B$ and $C$, but the values of $B$ and $C$ are equal, we should have $r_2 = (1, 3, 3)$. But taking the first vector as a reference vector, all species are now assigned label 1 and thus we would indeed end up with $r_2 = (1, 1, 1)$ and not $(1, 3, 3)$ as expected. So in this case, $r_1$ and $r_2$ would be treated as equal even though they are clearly different.

So these problems are the reason why we decided to omit ties and to break them randomly instead. However, after computing the Manhattan and Kendall tau distance, we checked if rankings that had been counted as identical before now led to a distance greater than zero and conversely, i.e. if we had obtained rankings with distance zero that had not been classified as identical. In total, we observed a difference in only 19 out of 4,000 trees, so we conclude that this simplification did not have a great impact on our results. However, finding a smarter way to deal with ties could be a goal for future work.

In total, we have seen that both investigated distance measures lead to similar results. We have also seen that ultrametricity of the underlying tree makes the rankings of all indices more similar – in the case of the original and the modified Shapley Values, we even get equality for ultrametric trees. However, for non-ultrametric trees, the rankings tend to differ more, and even though the different versions of the Shapley Value are highly correlated, surprisingly the probability of getting two identical rankings from these different versions for a given tree decreases as the number $n$ of taxa increases. Yet the normalized differences tend to zero, and the variability of the differences between the values gets smaller for increasing $n$.

We conclude that all biodiversity prioritization indices discussed in current literature, namely the Fair Proportion Index as well as all versions of the Shapely
Value, tend to give similar results, particularly if the number of species under consideration is large. As the Fair Proportion Index can be calculated most easily, we therefore think its wide use is justified. However, as the probability of getting identical rankings from different values is small for a large species set, we suggest that for biological data and real conservation decisions, more than one index should be taken into account.

It would be of interest to see if the differences in the rankings, which we observed for different kinds of random trees, also occur frequently on phylogenetic trees reconstructed from real data. This is another possible area for future research.

Acknowledgements  We want to thank Volkmar Liebscher for helpful comments on an earlier version of the manuscript.
References

Felsenstein J, Archie J, Day W, Maddison W, Meacham C, Rohlf F, Swofford D (2000) The newick tree format. URL http://evolution.genetics.washington.edu/phylip/newicktree.html

Fuchs M, Jin EY (2014) Equality of Shapley value and fair proportion index in phylogenetic trees. J Math Biol

Haake CJ, Kashiwada A, Su FE (2007) The Shapley value of phylogenetic trees. J Math Biol 56(4):479–497

Hartmann K (2012) The equivalence of two phylogenetic biodiversity measures: the Shapley value and Fair Proportion index. J Math Biol 67(5):1163–1170

Isaac NJ, Turvey ST, Collen B, Waterman C, Baillie JE (2007) Mammals on the EDGE: Conservation priorities based on threat and phylogeny. PLoS ONE 2(3):e296, DOI 10.1371/journal.pone.0000296

MATLAB (2013) version 8.1.0.604 (R2013a). The MathWorks Inc., Natick, Massachusetts

R Development Core Team (2014) R: A Language and Environment for Statistical Computing. R Foundation for Statistical Computing, Vienna, Austria, ISBN 3-900051-07-0

Stajich JE (2002) The bioperl toolkit: Perl modules for the life sciences. Genome Research 12(10):1611–1618, DOI 10.1101/gr.36102

Vos RA, Caravas J, Hartmann K, Jensen MA, Miller C (2011) Bio:: Phylo-phyloinformatic analysis using perl. BMC bioinformatics 12(1):63
