Many phylogenetic diversity indices are not robust to extinctions

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Abstract

Phylogenetic diversity indices provide a formal way to apportion evolutionary history amongst extant species. Understanding the properties of these measures is key to determining their applicability in conservation biology settings. In this short note, we investigate some questions posed in a recent paper [1]. In that paper, it is shown that under certain extinction scenarios, the ranking of the surviving species by their Fair Proportion index scores may be the reverse of their ranking beforehand. Our main result here shows that this behaviour extends to a large class of phylogenetic diversity indices. Next, we provide a necessary condition for reversals of Fair Proportion rankings to occur on phylogenetic trees whose edge lengths obey the ultrametric constraint. Lastly, while a direct analogue of the reversal result does not hold when using the Equal-Splits (ES) diversity index, nonetheless as few as two extinctions can lead to a complete ES ranking reversal on caterpillar trees. Specific examples of rooted phylogenetic trees displaying these behaviours are given.

Keywords: phylogenetic tree, biodiversity conservation, Fair Proportion index, Equal Splits index, phylogenetic diversity, species prioritization

1 Introduction

Each species on earth is the product of some evolutionary history, both unique to itself and shared with other species. Phylogenetic diversity indices are a family of measures that quantify this history, assigning to each species a numerical score based on their position in a phylogenetic tree. These diversity index scores

have found practical application in conservation biology. In particular, they have been used to suggest prioritisation rankings for biodiversity conservation [for example, see 2–5], often in conjunction with other measures.

However, conservation efforts take place at a time heavily impacted by extinctions of species [6] and these extinction events impact the very measures that conservation biologists use to try to prevent them. Figuratively speaking, extinctions remove branches from the tree of life, altering the phylogeny. This necessitates the recalculation of diversity index scores of surviving species, these measures being based on the phylogenetic tree structure. Since conservation programmes often employ large amounts of scarce resources [7] and require community buy-in [8], it is useful to know if and when extinction events could lead to recalculations that give markedly different priorities. Ideally, phylogenetic diversity indices would not only give informative prioritisation rankings but also be 'robust', that is, not particularly sensitive to changes caused by extinction events.

A recent paper [1] assesses the robustness of the Fair Proportion (FP) index on rooted phylogenetic trees. Those authors showed that rankings under the FP index can change markedly following certain extinction events. Furthermore, "for each phylogenetic tree, there are edge lengths such that the extinction of one leaf per cherry completely reverses the ranking" [1, p. 2]. In Section 3 here, after a section of preliminary definitions, we prove that analogous behaviour is exhibited by a much larger class of diversity indices.

Following Fischer et al., we initially place no constraint on the size of edge lengths required to obtain such a reversal. The examples contained in the original paper and the constructive methods appearing in the proofs of their Theorem 2 [1, Supp. Mat. pp. 2-15] and Theorem 2 here all tend to place the leaves at quite varied distances from the root vertex. This leads to natural questions about whether a similar result can be obtained when edge lengths obey an ultrametric constraint. In particular:

> "if we restrict the analysis to ultrametric trees where all leaves have the same distance to the root, what are the worst-case scenarios in this setting?" [1, p. 5]

By "worst-case" these authors refer to a combination of edge lengths and extinctions that re-orders the FP index score ranking as much as possible. In Section 4 we outline some necessary conditions for a complete reversal of FP index scores in the ultrametric context. Then we present examples of binary ultrametric phylogenetic trees for which FP index score rankings are reversible. This answers the question above by showing that the "worst-case scenario" on an ultrametric phylogenetic tree is as bad as possible.

We finish by investigating the robustness of another popular diversity index: the Equal-Spilts (ES) index. ES falls outside the family of diversity indices covered by Theorem 2 and we illustrate that this index is not always reversible under the same extinctions that reverse FP index score rankings. However, a necessary condition for ES ranking reversals (in terms of the

extinctions required) is given here and we show that for caterpillar trees such reversals can be caused by the extinction of just two species.

2 Preliminaries

Let X be a non-empty set of taxa (e.g. species), with $\mathsf{X} = n$. A *rooted binary phylogenetic X-tree* is a rooted tree $T = (V, E)$, where X is the set of leaves, and all edges are directed away from a distinguished root vertex ρ, and every non-leaf, non-root vertex has in-degree 1 and out-degree 2. All edges drawn in this paper will be directed down the page.

Let $P(T;\ \rho, v)$ be the path in T from the root ρ to $v \in V(T)$ (this path is unique if it exists). For any edge $e \in E(T)$, we write $x \in c_T(e)$ if $x \in X$ and $P(T;\ \rho, x)$ includes e. That is, $c_T(e)$ is the set (*cluster*) of leaves descended from the terminal vertex of e. For $v \in V(T)$, we also write $x \in c_T(v)$ if $x \in X$ and $P(T;\ \rho, x)$ includes v. If the (directed) edge (u, v) appears in a phylogenetic tree T, we say that u is the *parent* of v. If two distinct leaves x_1 and x_2 in X have the same parent vertex then we call $\{x_1, x_2\}$ a *cherry*, and a rooted binary phylogenetic tree with exactly one cherry is called a *caterpillar* tree. A *pendant* subtree of T is any subtree that does not contain the root vertex and is formed from T by the deletion of exactly one edge. Each binary phylogenetic tree has two *maximal* pendant subtrees formed by the deletion of an edge incident with the root.

We denote the two maximal pendant subtrees of tree T by T_a and T_b. The tree shape of T may be expressed in terms of these two maximal pendant subtrees by writing $T = (T_a, T_b)$. We may extend this notation to non-root non-leaf vertices of T, writing $T_a(v)$ and $T_b(v)$ for the maximal subtrees contained within the pendant subtree rooted at vertex v. The edge connecting the root vertex to T_a will be labelled a, the set of leaves in T_a will be denoted X_a, with $|X_a| = n_a$ and the number of cherries in T_a will be denoted c_a. Parallel notation applies to the subtree T_b and we write c_T for the total number of cherries in T. Figure 1 illustrates this notation.

The edges of every rooted binary phylogenetic tree considered in this paper are positively weighted. Let T be a rooted binary phylogenetic X-tree and let $\ell : E(T) \to \mathbb{R}^{>0}$ be a function that assigns a positive real-valued length $\ell(e)$ to each edge $e \in E(T)$. Suppose that $u, v \in V(T)$ are two vertices of T connected by a directed path from u to v. Then the *distance from u to v*, denoted $d(u, v)$, is the sum of the lengths of the edges in this path. If ℓ is such that for every two distinct leaves x and y we have $d(\rho, x) = d(\rho, y)$, we say that ℓ satisfies the *ultrametric* condition.

A (phylogenetic) *diversity index* on a rooted binary phylogenetic tree T is a function that assigns a portion of the total edge length of T to each species. This can be seen as partitioning the total evolutionary history (the *phylogenetic diversity* [9]) of a phylogenetic tree among its species. Loosely speaking, these functions allocate the value of each edge length among that edge's descendants

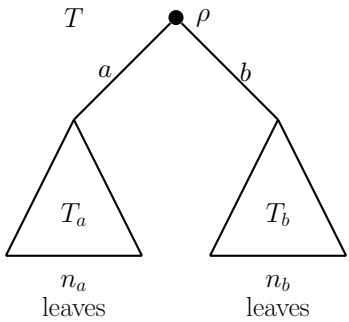


Fig. 1: Schematic diagram showing the notation for maximal pendant subtrees descended from the root vertex via edges a and b.

in such a way that respects the symmetries of the tree shape. We write φ_T to denote the diversity index φ applied to the phylogenetic tree T.

The formal definition of a diversity index builds on the related class of allocation functions [10]. Let $T = (V, E)$ be a rooted phylogenetic X-tree with edge length assignment function ℓ. An *allocation function* $\varphi_\ell : X \to \mathbb{R}^{\geq 0}$ is a real-valued function on the set of leaves of T that satisfies the following equation:

$$\sum_{x \in X} \varphi_\ell(x) = \sum_{e \in E} \ell(e) = PD(T, \ell),$$

and moreover it may be expressed as $\varphi_\ell(x) = \sum_{e \in E} \gamma(x, e)\ell(e)$, for every edge length assignment function ℓ, where all of the *coefficients* $\gamma(x, e)$ are non-negative.

A *diversity index* (on T) is an allocation function $\varphi_\ell : X \to \mathbb{R}^{>0}$ given by $\varphi_\ell(x) = \sum_{e \in E} \gamma(x, e)\ell(e)$ for every edge length assignment function ℓ, that additionally satisfies the conditions (DI_1) and (DI_2) below:

- (DI_1) *Descent condition:* $\gamma(x, e) = 0$ if x is not descended from e.
- (DI_2) *Neutrality condition:* The coefficients $\gamma(x, e)$ are a function of the tree shape of P_e. Moreover, suppose that P_e and P_f are pendant subtrees of T with the same tree shape. If the leaves x in P_e and y in P_f appear in corresponding positions in their respective subtrees, then $\gamma(x, e) = \gamma(y, f)$.

Two diversity indices are of particular importance: the Fair Proportion (or Evolutionary Distinctiveness) index [2, 11] and the Equal-Splits index [11, 12]. For each leaf $x \in X$, the *Fair Proportion* (FP) index of x in T is given by

$$FP_T(x) = \sum_{e \in P(T;\, \rho, x)} \frac{\ell(e)}{|c_T(e)|}.$$

As every phylogenetic tree considered in this paper is binary, we use the following particular formulation of the ES index. For each leaf $x \in X$, the (binary)

Equal-Splits (ES) index of x in T is given by

$$ES_T(x) = \sum_{e \in P(T;\ \rho, x)} \frac{\ell(e)}{2^p},$$

where p is the number of edges between e and x in the path $P(T;\ \rho, x)$.

Furthermore, we use, and repeat here, the definitions of *ranking*, *strict*, and *reversible* as they appear in [1] (pp. 2,3). A *ranking* $\pi(S, f)$ for a set $S = \{s_1, \ldots, s_n\}$ based on a function $f : S \to \mathbb{R}$ is an ordered list of the elements of S such that $f(s_i) \geq f(s_j)$ if and only if s_i appears before s_j in π. A ranking $\pi(S, f)$ is called *strict* if none of the values in S are equal. A ranking π_T is called *reversible* for diversity index φ if there is a subset X' of X whose removal from T leads to an induced subtree $\tilde{T}$ whose corresponding ranking $\pi_{\tilde{T}} = \pi(X \backslash X', \varphi_{\tilde{T}})$ ranks the species in the opposite order to the ranking $\pi_T = \pi(X \backslash X', \varphi_T)$. We write $\tilde{X} = \{\tilde{x}_1, \tilde{x}_2, \ldots, \tilde{x}_t\}$ for the t species that survive an extinction event. The induced subtree $\tilde{T}$ is the minimal subtree of T that spans $\tilde{X}$ and the root vertex.

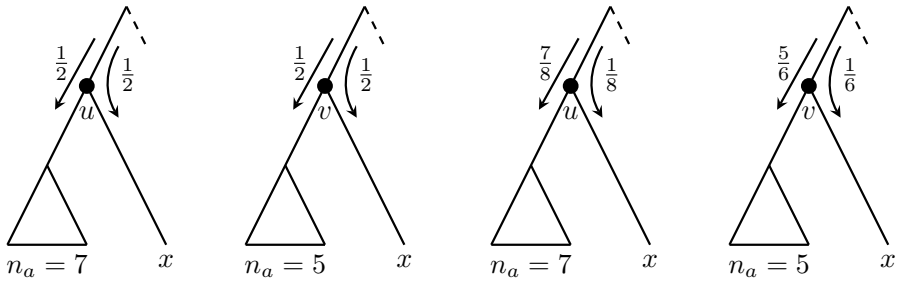
For the diversity index $\varphi(x) = \sum_{e \in E} \gamma(x, e)\ell(e)$, the *ratio of allocation* at vertex v is given by $\sum_{x \in T_a(v)} \gamma(x, e) : \sum_{x \in T_b(v)} \gamma(x, e)$. Each diversity index may be characterised by its ratios of allocation. Non-root non-leaf vertices may be categorised by the equivalence relation $\sim$. For $u, v \in V(T)$, write $u \sim v$ if and only if the multiset of tree shapes $\{T_1(u), T_2(u)\}$ is the same as the multiset of tree shapes $\{T_1(v), T_2(v)\}$.

Two types of diversity index will be considered further, defined in terms of their ratios of allocation. An *interior diversity index* is a diversity index where no ratio of allocation is a $0 : 1$ or $1 : 0$ ratio. Equivalently, a diversity index φ given by $\varphi(x) = \sum_{e \in E} \gamma(x, e)\ell(e)$ is interior if and only if $\gamma(x, e)$ is strictly positive whenever x is descended from e. We call any diversity index that is not interior a *boundary* diversity index. These names refer to the position of a diversity index in the compact convex space $S(T, \ell)$ of diversity indices on the tree T under edge length assignment ℓ (see [10]).

For a rooted phylogenetic tree T, let a *singular* $\sim$-equivalence class be one whose representative vertex is the root of a pendant subtree of T that itself contains a maximal pendant subtree consisting of a single leaf. In Figure 2, u and v are both representatives of singular $\sim$-equivalence classes. A *rigid diversity index* is a diversity index where the ratio of allocation is the same for at least two singular $\sim$-equivalence classes that contain different numbers of leaves. Figure 2 illustrates that Equal-Splits is rigid whereas Fair Proportion is not rigid.

3 Main results

In this section we show that Theorem 2 of [1] can be extended beyond the Fair Proportion index to apply to every non-rigid interior diversity index (Theorem 2 below). Let φ be such a diversity index. Our inductive proof of this result



(a) Equal-Splits (b) Fair Proportion

Fig. 2: (a) The Equal-Splits index is a rigid diversity index, as the ratio of allocation is unchanged from u to v although the number of leaves in the left-hand subtree (represented by a triangle) is changed. (b) In contrast, the Fair Proportion index is not a rigid diversity index, as can be seen from the different ratio of allocation in each case.

relies on building up a collection of edge lengths for a phylogenetic tree T based upon edge lengths that make φ reversible on maximal subtrees T_a and T_b. We begin with Lemma 1, a result that allows us to adjust the initial edge lengths in a useful way before starting the construction given in the proof of Theorem 2.

Lemma 1 *Let $T = (T_a, T_b)$ be a rooted binary phylogenetic X-tree and let $\varphi_T = \sum_{e \in E(T)} \gamma_T(x, e)\ell(e)$ be an interior diversity index on T that is not rigid. Suppose that $|X_a| \geq 2$ and that φ induces a strict and reversible ordering of taxa in $\tilde{X}_a \subset X_a$ after the extinction of one leaf per cherry of T_a. Then there exist edge lengths for T such that $\varphi_T(\tilde{x}_i) \neq \varphi_{\tilde{T}}(\tilde{x}_j)$ for all $\tilde{x}_i$ and $\tilde{x}_j$ in $\tilde{X}_a$.*

Proof Let T be as drawn in Figure 1 and let $\tilde{X}_a$ be indexed such that $\varphi_{T_a}(\tilde{x}_1) < \ldots < \varphi_{T_a}(\tilde{x}_{n_a - c_a})$. We prove the result by describing how the edge lengths of T_a that allow the ranking reversal on $\tilde{X}_a$ can be adjusted to give distinct φ index scores.

First, assume that $\tilde{x}_i$ is a leaf with $\varphi_T(\tilde{x}_i) = \varphi_{\tilde{T}}(\tilde{x}_i)$. As φ induced a strict and reversible ranking, $\tilde{x}_i$ is the only leaf for which this equality holds. Let e_i be the pendant edge incident to $\tilde{x}_i$ in T and let e_i^+ be the edge in T whose terminal vertex is the parent of $\tilde{x}_i$. Suppose that e_i^+ is edge a, incident with the root of T. Since φ is an interior diversity index $\gamma_T(\tilde{x}_i, e_i^+)$ and $\gamma_{\tilde{T}}(\tilde{x}_i, e_i^+)$ are both strictly positive. Moreover, as φ is not rigid we have $\gamma_T(\tilde{x}_i, e_i^+) \neq \gamma_{\tilde{T}}(\tilde{x}_i, e_i^+)$. But then

$$\varphi_T(\tilde{x}_i) = \ell(e_i) + \gamma_T(\tilde{x}_i, e_i^+)\ell(e_i^+) \neq \ell(e_i) + \gamma_{\tilde{T}}(\tilde{x}_i, e_i^+)\ell(e_i^+) = \varphi_{\tilde{T}}(\tilde{x}_i),$$

contradicting our supposition.

Hence it must be the case that e_i^+ is within T_a. Extending e_i^+ will increase $\varphi_{T_a}(\tilde{x}_i)$ and $\varphi_{\tilde{T}_a}(\tilde{x}_i)$ by different amounts because φ is not rigid. Specifically, we choose to extend e_i^+ by the lesser of $\frac{1}{2}\left[\varphi_{T_a}(\tilde{x}_{i+1}) - \varphi_{T_a}(\tilde{x}_i)\right]$ and $\frac{1}{2}\left[\varphi_{\tilde{T}_a}(\tilde{x}_{i-1}) - \varphi_{\tilde{T}_a}(\tilde{x}_i)\right]$ (or

the defined value from these two choices if only one exists). This particular choice is small enough to ensure that neither the π_a ranking nor the $\tilde{\pi}_a$ ranking is altered by the extension. Hence strict reversibility is maintained. Moreover, extending e_i^+ in such a manner ensures that $\varphi_T(\tilde{x}_i)$ and $\varphi_{\tilde{T}}(\tilde{x}_i)$ will have distinct values.

Second, assume that $\tilde{x}_i$ and $\tilde{x}_j$ are distinct leaves with $\varphi_T(\tilde{x}_i) = \varphi_{\tilde{T}}(\tilde{x}_j)$. Then we can extend e_i, the pendant edge incident to $\tilde{x}_i$, by the lesser of $\frac{1}{2}\left[\varphi_{T_a}(\tilde{x}_{i+1}) - \varphi_{T_a}(\tilde{x}_i)\right]$ and $\frac{1}{2}\left[\varphi_{\tilde{T}_a}(\tilde{x}_{i-1}) - \varphi_{\tilde{T}_a}(\tilde{x}_i)\right]$ (or the defined value from these two choices if only one exists). Extending the pendant edge incident to $\tilde{x}_i$ increases both $\varphi_T(\tilde{x}_i)$ and $\varphi_{\tilde{T}}(\tilde{x}_i)$ by the same amount but does not alter $\varphi_{\tilde{T}}(\tilde{x}_j)$. This particular choice is small enough to ensure that neither the π_a ranking nor the $\tilde{\pi}_a$ ranking is altered by the extension. Hence strict reversibility is maintained. Moreover, extending the pendant edge incident to $\tilde{x}_i$ in such a manner ensures that $\varphi_T(\tilde{x}_i)$ and $\varphi_{\tilde{T}}(\tilde{x}_j)$ will have distinct values. We repeat this step as necessary for every such pair of leaves.

Finally, we choose $\ell(a)$ to be short enough to ensure that it is less than the smallest difference between any two φ_{T_a}- or $\varphi_{\tilde{T}_a}$-index scores from our modified version of T_a. So even if one leaf were to be allocated the entire length of edge a, the ranking orders π_a and $\tilde{\pi}_a$ would not change.

Therefore, given a set of edge lengths for T, we can adjust them in the manner described above to ensure $\varphi_T(\tilde{x}_i) \neq \varphi_{\tilde{T}}(\tilde{x}_j)$ for all $\tilde{x}_i$ and $\tilde{x}_j$ in $\tilde{T}_a$. □

We turn now to the main result of the paper. Theorem 2 extends Theorem 2 of [1] to diversity indices beyond the Fair Proportion index. It shows that a large proportion diversity indices are reversible in the same sense as Fair Proportion (i.e. after a one-per-cherry extinction event), with only rigid and boundary diversity indices not being reversible in this way.

Theorem 2 *Let $n \geq 2$ and let $T = (T_a, T_b)$ be a rooted binary phylogenetic X-tree with $|X| = n$. Let $\tilde{T}$ be the induced $\tilde{X}$-tree that results from we deleting one leaf out of each cherry of T. Then, for any non-rigid interior diversity index φ, there exists an edge length assignment function ℓ on T such that there is a strict φ ranking π_T for the leaves of T that is reversible with respect to $\tilde{T}$ and such that $\tilde{X}$ contains the species that has the highest φ index score in T.*

Proof We proceed by induction on n. As a base case we consider a rooted phylogenetic tree with exactly two leaves and two edges of different lengths. If the taxon incident with the shortest of the two edges is deleted, then the remaining taxon is in a strict and reversible ordering (of size one) and the result holds.

Next, for the inductive step assume that the theorem holds for the non-rigid interior diversity index φ on all rooted phylogenetic trees with less than n leaves. Let $T = (T_a, T_b)$ be a rooted phylogenetic tree with n leaves, as drawn in Figure 1. Without loss of generality we have $n_a \geq n_b$. We show that by using the edge lengths that allowed reversible orderings of φ on T_a and T_b, we are able to choose edge lengths that make φ reversible on T as a whole.

As T_a has less than n leaves, the extinction of one leaf per cherry induces a strict and reversible ranking π_a on the leaves of T_a. Let $\tilde{X} = \{\tilde{x}_1, \ldots, \tilde{x}_{n-c_T}\}$ be the set

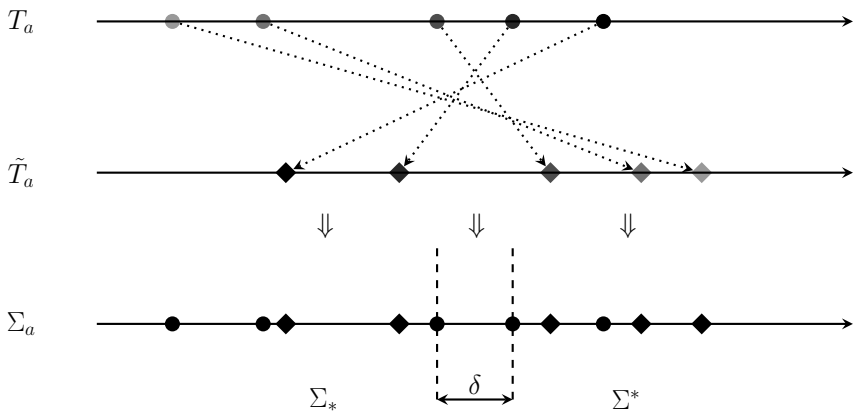


Fig. 3: Illustration of the first part of the construction described in the proof of Theorem 2. Each horizontal line represents the set of real numbers. Dotted lines indicate the reversal of index scores of leaves in T_a after one extinction per cherry, as per our induction hypothesis. The scores for both T_a and $\tilde{T}_a$ are combined on the bottom number line, where, by Lemma 1, the $2(n_a - c_a)$ scores may be made distinct without affecting the initial reversal. Finally the edge lengths of subtree T_b are adjusted and scaled to fit the index scores into the interval of size δ between the vertical dashed lines.

of leaves that is not deleted, labelled such that $\{\tilde{x}_1, \ldots, \tilde{x}_{n_a - c_a}\}$ is contained in T_a and $\{\tilde{x}_{n_a - c_a + 1}, \ldots, \tilde{x}_{n - c_T}\}$ is contained in T_b. Relabelling if necessary, we have

$$\varphi_{T_a}(\tilde{x}_1) < \varphi_{T_a}(\tilde{x}_2) < \ldots < \varphi_{T_a}(\tilde{x}_{n_a - c_a})$$

and

$$\varphi_{\tilde{T}_a}(\tilde{x}_1) > \varphi_{\tilde{T}_a}(\tilde{x}_2) > \ldots > \varphi_{\tilde{T}_a}(\tilde{x}_{n_a - c_a}).$$

As described in Lemma 1, we choose a small value for $\ell(a)$ that does not alter any of these inequalities. We construct a set of combined φ index scores for $\tilde{X}$ from both T and $\tilde{T}$, denoted $\Sigma_a \subset \mathbb{R}^{>0}$. In particular:

$$\Sigma_a = \{\varphi_T(\tilde{x}_i) | i \in 1, \ldots, n_a - c_a\} \cup \{\varphi_{\tilde{T}}(\tilde{x}_i) | i \in 1, \ldots, n_a - c_a\}.$$

By Lemma 1, since φ is non-rigid and interior, each element of Σ_a can be made to have a unique value by adjusting edge lengths within T_a. Moreover, this is achievable in a way that the ranking π_T restricted to T_a is the same as π_a. Thus we are able to ensure that Σ_a contains $2(n_a - c_a)$ distinct positive real numbers. See Figure 3 for an illustration of this construction.

Let Σ_* be the subset of Σ_a containing the $n_a - c_a$ least elements of Σ_a under the usual ordering of real numbers and let Σ^* be the subset of Σ_a containing the $n_a - c_a$ greatest elements of Σ_a under the same ordering. Hence, Σ_a is the disjoint union of Σ_* and Σ^*.

Next we consider the remaining taxa of T. The subtree T_b has less than n leaves and hence the extinction of one leaf per cherry induces a strict and reversible ranking π_b on $\tilde{X}_b$. Similar to T_a, relabelling if necessary, we have

$$\varphi_{T_b}(\tilde{x}_{n_a - c_a + 1}) < \varphi_{T_b}(\tilde{x}_{n_a - c_a + 2}) < \ldots < \varphi_{T_b}(\tilde{x}_{n - c_T})$$

and

$$\varphi_{\tilde{T}_b}(\tilde{x}_{n_a-c_a+1}) > \varphi_{\tilde{T}_b}(\tilde{x}_{n_a-c_a+2}) > \ldots > \varphi_{\tilde{T}_b}(\tilde{x}_{n-c_T}).$$

Similar to the T_a case, we choose a small enough value for $\ell(b)$ so that the above rankings are maintained. We construct the set

$$\Sigma_b = \{\varphi_T(\tilde{x}_i) | i \in n_a - c_a + 1, \ldots, n - c_T\} \cup \{\varphi_{\tilde{T}}(\tilde{x}_i) | i \in n_a - c_a + 1, \ldots, n - c_T\},$$

but in contrast to Σ_a do not require that Σ_b contains $2(n_b - c_b)$ distinct values. However, we do note that because φ is an interior diversity index, every member of Σ_b is strictly positive.

Now let $\delta = \min \Sigma^* - \max \Sigma_*$ be the size of the gap between the two halves of Σ_a (see Figure 3). We uniformly multiply the lengths of edges in $E(T_b) \cup \{b\}$ by a positive real constant c, chosen so that $c\,(\max \Sigma_b) < \delta$. That is, we scale (down) the entirety of T_b as well as edge b such that the range of values in the rescaled Σ_b extends less than δ. (In practice it may be tidier to scale up T_a and a to achieve the same result.) Call the resulting subtree T_b'. Finally, to each pendant edge in T_b' add the value of $\max \Sigma_*$. This shifts the index scores of T_b' into the gap between Σ_* and Σ^* without altering the ranking of these leaves.

Let $\tilde{x}_\alpha$ be the taxon such that $\varphi_{T_a}(\tilde{x}_\alpha)$ is the largest value in Σ_* among scores from T_a (as opposed to scores from $\tilde{T}_a$). Then the result of the above construction is that we have

$$\begin{aligned}\varphi_T(\tilde{x}_1) < \ldots < \varphi_T(\tilde{x}_\alpha) < \varphi_T(\tilde{x}_{n_a-c_a+1}) \\ < \ldots < \varphi_T(\tilde{x}_{n-c_T}) < \varphi_T(\tilde{x}_{\alpha+1}) < \ldots < \varphi_T(\tilde{x}_{n_a-c_a})\end{aligned}$$

and

$$\begin{aligned}\varphi_{\tilde{T}}(\tilde{x}_1) > \ldots > \varphi_{\tilde{T}}(\tilde{x}_\alpha) > \varphi_{\tilde{T}}(\tilde{x}_{n_a-c_a+1}) \\ > \ldots > \varphi_{\tilde{T}}(\tilde{x}_{n-c_T}) > \varphi_{\tilde{T}}(\tilde{x}_{\alpha+1}) > \ldots > \varphi_{\tilde{T}}(\tilde{x}_{n_a-c_a}).\end{aligned}$$

Therefore the extinction of $X - \tilde{X}$ has induced a strict a reversible ranking on $\tilde{X}$ given our chosen edge lengths. Hence the induction is proved and the theorem holds for all $n \geq 2$. □

3.1 Rigid interior diversity indices

For a ranking derived from a rigid interior diversity index to undergo a strict reversal, the extinction of at least one leaf per cherry is still required, as the proof of Theorem 1 in [1] extends directly to diversity indices in general. However, as an examination of the ES index will show, a one-per-cherry extinction event may not be enough to reverse all of the survivors' index scores. We would like to know how few extra extinctions could induce a ranking reversal. Let T be a phylogenetic tree rooted at ρ and let $x \in X$ be a leaf vertex with parent $v \in V(T)$ distinct from ρ. Then we call x an *isolated leaf* if there is no vertex u in the path $P(T;\ \rho, v)$, excluding possibly ρ, such that u itself is the parent of a leaf vertex. Proposition 3 shows that in addition to one taxon per cherry, we additionally require all but one isolated leaf to go extinct before a strict and reversible ranking on T can occur for rigid interior diversity indices.

Proposition 3 *Let T be a rooted phylogenetic X-tree with $|X| \geq 3$ and let φ be a rigid diversity index on T. Suppose π_T is a strict and reversible ranking concerning*

the φ diversity index for T with respect to $\tilde{X}$ and induced subtree $\tilde{T}$. Then $X' = X - \tilde{X}$ contains at least one leaf from each cherry of T and at least all but one of the isolated leaves of T. In the case that one of the maximal pendant subtrees of T contains a single leaf then X' must contain all of the isolated leaves of T.

Proof Let a *fixed leaf* for $\tilde{X}$ be any leaf x in $\tilde{X}$ where $\varphi_T(x) = \varphi_{\tilde{T}}(x)$. For the extinction of X' to induce a strict and reversible ranking on $\tilde{X}$ there can be at most one fixed leaf for $\tilde{X}$. Each isolated vertex may be a fixed leaf if φ is a rigid diversity index. Any leaf whose parent vertex is the root is also a fixed leaf. Therefore, to induce a strict and reversible ranking on $\tilde{X}$, the deletion of at least all but one isolated vertex is required and if one of the maximal pendant subtrees of T contains a single leaf the final isolated vertex must be deleted too. Since the extinction of at least one leaf per cherry is needed to reverse any diversity index ranking, the result is shown. □

We do not show that the additional extinction of isolated vertices is sufficient to cause a reversal for any rigid diversity index. However, we consider further the special case of the reversal of ES index score rankings on the family of caterpillar trees.

Corollary 4 *Let T be a rooted caterpillar tree with at least four leaves. Then the extinction of one leaf from the cherry of T is necessary, but not sufficient, to cause a strict ranking of Equal Splits index scores to reverse.*

Moreover, let $X = \{x_1, x_2, x_3, \ldots, x_n\}$ be the leaves of T, where x_n is adjacent to the root vertex, and there is a path of length two from the root vertex to x_{n-1}. Then the extinction of any strict subset of $\{x_1, x_2, x_3, \ldots, x_{n-2}\}$ cannot cause a strict ranking of Equal-Splits index scores to reverse.

Proof Let x_1 and x_2 be the two distinct leaves that form the unique cherry of T. By Theorem 1 in [1], it is necessary for at least one of x_1, x_2 to be deleted for the ranking of ES index scores to reverse.

The extinction of, say, x_1 alone will lead to an increase in the ES index score of x_2, but the ES index scores of all other vertices remain the same. If T contains at least four leaves, there are at least two leaves whose index scores are unaffected, and hence their ranking order does not reverse. Thus the extinction of x_1 or x_2 alone is not enough to reverse the ES index scores.

For a rooted caterpillar tree with n leaves, suppose a strict subset of $\{x_1, x_2, x_3, \ldots, x_{n-2}\}$ becomes extinct. Note that the extinction of a leaf x_i affects the ES index score of precisely those leaves descended from the parent of x_i and no others. By this reasoning the ES index scores of x_{n-1} and x_n are unaffected by such an extinction and the ranking cannot reverse. Therefore the deletion of x_{n-1} or x_n is necessary for an ES ranking reversal. □

We give an example of edge lengths for which the extinction of two species may induce an ES ranking reversal. Consider the rooted caterpillar tree Cat_n

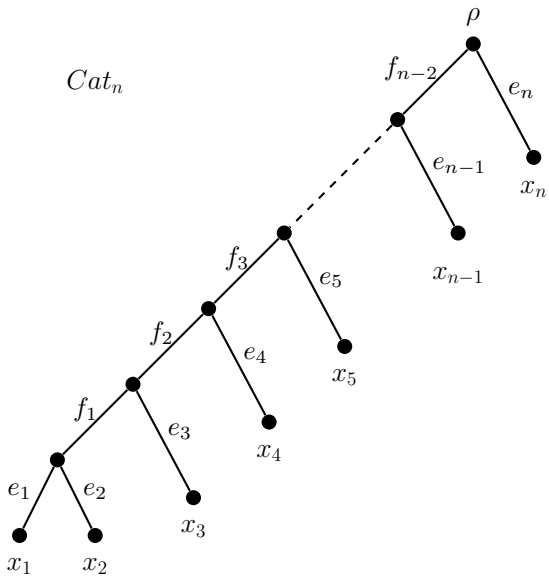


Fig. 4: A general caterpillar tree used to show that ES index score rankings can be reversed with as few as two extinctions.

in Figure 4, where $n \geq 4$. Let the edges of Cat_n be assigned lengths by the function $\ell : E(Cat_n) \to \mathbb{R}$ as follows:

- $\ell(e_1) = \ell(e_2) = \ell(e_{n-1}) = 1$
- $\ell(e_i) = 2^{i-2} + n - i - 1$, for $3 \leq i \leq n-2$
- $\ell(e_n) = 2^{n-2} + n - 3$
- $\ell(f_i) = 2^{n-2}$, for all $1 \leq i \leq n-2$

Then suppose that leaves x_1 and x_{n-1} are deleted and that $\tilde{Cat}_n$ is the resulting phylogenetic tree. Table 1 shows the ES index scores for Cat_n and $\tilde{Cat}_n$, illustrating the ranking reversal. In the case $n = 10$, the values for $e_1, e_2, \ldots, e_{10}$ are $1, 1, 8, 9, 12, 19, 34, 65, 1$, and 263, and $f_i = 256$ for the values $1 \leq i \leq 8$. The index scores for this case scenario appear in Table 1.

4 Robustness of diversity indices under the ultrametric constraint

In this section we consider the rankings of diversity index scores on phylogenetic trees whose edge lengths obey the ultrametric constraint. We note that for every diversity index φ the ranking $\pi(X, \varphi_T)$ on an ultrametric rooted phylogenetic X-tree T cannot be strict, as both leaves from any ultrametric cherry have equal index scores. With this in mind, we impose some further conditions that are not explicitly addressed by the earlier definition of a reversible diversity index.

x	$ES_{Cat_n}(x)$	$n = 10$	$ES_{\tilde{Cat}_n}(x)$	$n = 10$
x_2	2^{n-2}	256	$\mathbf{2^{n-1} + 1}$	**513**
x_{n-2}	$2^{n-2} + 1$	257	$2^{n-2} + 2^{n-4} + 1$	321
x_{n-3}	$2^{n-2} + 2$	258	$2^{n-2} + 2^{n-5} + 2$	290
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
x_5	$2^{n-2} + n - 6$	260	$2^{n-2} + 2^3 + n - 6$	268
x_4	$2^{n-2} + n - 5$	261	$2^{n-2} + 2^2 + n - 5$	265
x_3	$2^{n-2} + n - 4$	262	$2^{n-2} + 2^1 + n - 4$	264
x_n	$\mathbf{2^{n-2} + n - 3}$	**263**	$2^{n-2} + n - 3$	263

Table 1: Reversal of ES index scores for the n-leaf caterpillar tree Cat_n under the extinction of x_1 and x_{n-1}. Calculated index scores are provided for n in general and the case where $n = 10$. The largest value in each column appears in boldface.

Whenever $\pi_T(x_i) < \pi_T(x_j)$, we require $\pi_{\tilde{T}}(x_i) > \pi_{\tilde{T}}(x_j)$ for $\pi_{\tilde{T}}$ to be considered to be in the opposite order to π_T. That is, it is not enough for $\pi_{\tilde{T}}(x_i) = \pi_{\tilde{T}}(x_j)$. Moreover, to eliminate trivial reversals, for a ranking $\pi_{\tilde{T}}$ to be considered to be in the opposite order to π_T, we require $\pi_T(x_i) < \pi_T(x_j)$ and $\pi_{\tilde{T}}(x_i) > \pi_{\tilde{T}}(x_j)$ for at least one pair of distinct leaves x_i, x_j. We now outline some necessary conditions for the reversibility of FP index scores in the ultrametric context.

Proposition 5 *Let T be a rooted binary phylogenetic X-tree whose edge lengths satisfy the ultrametric condition and let π_T be the ranking of FP index scores for T. Suppose $x \in X$ is a leaf vertex contained in no cherry of T. Let v be the parent vertex of x and write $c_T(v)$ as the disjoint union $\{x\} \cup A$, where A contains at least two distinct leaves of T.*

Then there exist ultrametric edge lengths and a set of extinctions for which the ranking π_T is reversible only if, whenever x survives, the entire set A has become extinct.

Proof Let $x \in X$ be a leaf of T that is not contained in any cherry, and let v be the parent vertex of x. As x is not in a cherry, $c_T(v)$ must contain at least two distinct leaf vertices different from x, say y and z.

Then $FP_T(x)$ must be larger than $FP_T(y)$. To see this, first note that both x and y are allocated the same proportion of edge lengths along the path from the root vertex to v. As T satisfies the ultrametric condition, the length of edge (v, x)

is the same as the length of the path between v and y. Yet while leaf x is allocated the entire length of edge (v, x), leaf y is only allocated part of the total length of the edges along the path from v to y. This is because y must share some of this total with z (from along the edges connecting v to the common parent of y and z).

Next, suppose a set of extinctions occurs that both x and y survive and that $\tilde{T}$ is the resulting phylogenetic tree. Then $FP_{\tilde{T}}(y)$ can be no larger than $FP_{\tilde{T}}(x)$, with equality holding if and only if x and y form a cherry in $\tilde{T}$. Hence x and y are not ranked in the opposite order in $\pi_{\tilde{T}}$ compared to π_T. Hence the ranking π_T is not reversible if y survives alongside x. Repeating this observation for all vertices in $c_T(v)$ (other than x) gives the stated result. □

Corollary 6 *Let T be a rooted binary phylogenetic X-tree whose edge lengths satisfy the ultrametric condition and let π_T be the ranking of FP index scores for T. There exist ultrametric edge lengths and a one-per-cherry extinction event for which the ranking π_T is reversible only if every leaf in X is a member of some cherry.*

Proof Let $x \in X$ be a leaf of T that is not contained in any cherry, and let v be the parent vertex of x. As x is not in a cherry, $c_T(v)$ must contain at least two distinct leaf vertices different from x.

Choose two vertices from $c_T(v)$ that form a cherry, say y and z. Suppose that, say, y survives a one-per-cherry extinction event. Since x is not contained in any cherry of T, then x must also survive the extinction event. Therefore, by Proposition 5, the ranking π_T is not reversible. □

5 Examples of ultrametric phylogenetic X-trees with reversible rankings

We present a family of ultrametric rooted phylogenetic trees with reversible rankings. Moreover we give specific edge lengths such that both the Fair Proportion and Equal Splits indices are reversible after the extinction of one leaf per cherry. Further examples are provided in supplementary material. The family is illustrated by a representative in Fig. 5a, where $n = 12$. A similar tree can be constructed for any even number of leaves n, where the sum of the edges lengths on the unique path from the root vertex to a leaf is $n - 1$. A second reversible ultrametric family, of balanced phylogenetic X-trees, is presented in supplementary material. Edge lengths for both families are specified so that a one-per-cherry extinction event induces both an ES and FP ranking reversal.

Let U be the rooted phylogenetic tree in Fig. 5a with edge lengths as marked. The tree $\tilde{U}$ in Fig. 5b is obtained from U after the extinction of every species with an even subscript. The Fair Proportion and Equal-Splits index scores for each surviving leaf are given in Table 2. Let π_U and $\pi_{\tilde{U}}$ be rankings of FP index scores for the trees U and $\tilde{U}$ respectively. Observe that $\pi_{\tilde{U}}$ ranks the species in the opposite order to π_U, hence π_U is reversible. (The scores of leaves x_1 and x_3 remain equal before and after the extinctions.)

x	$FP_U(x)$	$FP_{\tilde{U}}(x)$	$ES_U(x)$	$ES_{\tilde{U}}(x)$
x_1	**6.642**	8.283	**6.469**	7.938
x_3	**6.642**	8.283	**6.469**	7.938
x_5	6.392	8.783	6.438	8.875
x_7	6.225	9.450	6.375	9.750
x_9	6.100	10.200	6.250	10.500
x_{11}	6.000	**11.000**	6.000	**11.000**

Table 2: Fair Proportion and Equal-Splits index values for U and $\tilde{U}$, rounded to three decimal places. The largest value in each column appears in boldface.

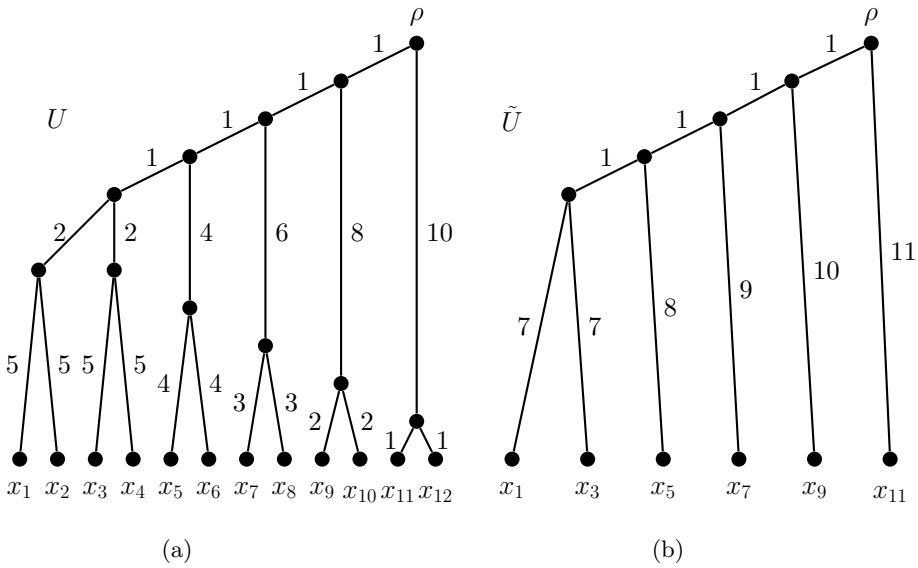


Fig. 5: An ultrametric rooted phylogenetic tree U before and after a set of extinctions that reverses both the FP and ES index score rankings for surviving species.

6 Concluding remarks

The potential for the reversal of rankings based on diversity index scores could cause uncertainty over the usefulness of these measures. [1] did not conclude that reversibility was grounds for disregarding the use of the Fair Proportion index entirely, but that it was an effect that needed to be kept in mind. Based

on Theorem 2 here, we suggest that this behaviour is an unavoidable part of using phylogenetic diversity indices in general, apart from some boundary cases that seem quite unrealistic. As such, reversibility is less a property to be held against FP in preference to other potential diversity indices and rather more an aspect of using this type of measure in general. We should not be surprised that a species' contribution to the phylogenetic diversity of a larger set increases given the extinction of close relatives. Thus a diversity index that sensibly measures this contribution cannot be expected to fix its scores in the face of ongoing extinction events. Combinations of extinctions will likely lead to many score increases (of differing magnitudes) that could upset the initial ranking.

The examples given in this paper have shown that ranking reversals may be induced not only given quite varied edge lengths but also on rooted phylogenetic trees under the ultrametric constraint. It may be useful for further investigation to determine the minimum number of extinctions required to cause a FP ranking reversal on ultrametric trees. This number will likely depend on the total number of leaves in a tree, as well as the number of leaves allowed to have the same FP index score despite not sharing a cherry. An understanding of these minimal extinction events could help to determine whether the converse of Proposition 5 holds and the extent to which real, time-based phylogenies may be susceptible to reversals.

Phylogenetic diversity indices, as have been used until now and as were described in [10], have been based on the assumption that, while edge lengths are used to calculate particular score values, the method of calculation should be independent of the edge lengths. This has not been adequately justified apart from on the grounds of mathematical simplicity and the fact that the two diversity indices used in practice (FP and ES) both have this property. The widespread nature of diversity index ranking reversals suggests there may be value in using a measure that takes into account edge lengths more directly, if doing so could minimise this behaviour.

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References

[1] Fischer, M., Francis, A., Wicke, K.: Phylogenetic diversity rankings in the face of extinctions: The robustness of the fair proportion index. Systematic Biology (2022)

[2] Isaac, N.J., Turvey, S.T., Collen, B., Waterman, C., Baillie, J.E.: Mammals on the edge: conservation priorities based on threat and phylogeny. PloS One **2**(3), 296 (2007)

[3] Bordewich, M., Rodrigo, A.G., Semple, C.: Selecting taxa to save or sequence: desirable criteria and a greedy solution. Systematic biology **57**(6), 825–834 (2008)

[4] Jetz, W., Thomas, G.H., Joy, J.B., Redding, D.W., Hartmann, K., Mooers, A.O.: Global distribution and conservation of evolutionary distinctness in birds. Current Biology **24**, 919–930 (2014)

[5] Forest, F., Moat, J., Baloch, E., Brummitt, N.A., Bachman, S.P., Ickert-Bond, S., Hollingsworth, P.M., Liston, A., Little, D.P., Mathews, S., *et al.*: Gymnosperms on the edge. Scientific reports **8**(1), 1–11 (2018)

[6] Davis, M., Faurby, S., Svenning, J.-C.: Mammal diversity will take millions of years to recover from the current biodiversity crisis. Proceedings of the National Academy of Sciences USA **115**, 11262–11267 (2018)

[7] White, T.B., Petrovan, S.O., Christie, A.P., Martin, P.A., Sutherland, W.J.: What is the price of conservation? A review of the status quo and recommendations for improving cost reporting. BioScience **72**(5), 461–471 (2022)

[8] Griffiths, R., Bell, E., Campbell, J., Cassey, P., Ewen, J., Green, C., Joyce, L., Rayner, M., Toy, R., Towns, D., Wade, L., Walle, R., Veitch, C.: Costs and benefits for biodiversity following rat and cat eradication on Te Hauturu-o-Toi/Little Barrier Island. In: Veitch, C.R., Clout, M.N., Martin, A.R., Russell, J.C., West, C.J. (eds.) Island Invasives: Scaling up to Meet the Challenge. Occasional Paper SSC, pp. 558–567. IUCN, Gland, Switzerland (2019)

[9] Faith, D.P.: Conservation evaluation and phylogenetic diversity. Biological Conservation **61**, 1–10 (1992)

[10] Manson, K., Steel, M.: Spaces of phylogenetic diversity indices: Combinatorial and geometric properties. Bulletin of Mathematical Biology **85** (2023)

[11] Redding, D.: Incorporating genetic distinctness and reserve occupancy into a conservation priorisation approach. Master's thesis: University of East Anglia (2003)

[12] Redding, D.W., Mazel, F., Mooers, A.Ø.: Measuring evolutionary isolation for conservation. PLoS One **9**(12), 113490 (2014)