

Formal Links between Feature Diversity and Phylogenetic Diversity

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ABSTRACT

1 The extent to which phylogenetic diversity (PD) captures feature diversity (FD) is a
2 topical and controversial question in biodiversity conservation. In this short paper, we
3 formalise this question and establish a precise mathematical condition for FD (based on
4 discrete characters) to coincide with PD. In this way, we make explicit the two main
5 reasons why the two diversity measures might disagree for given data; namely, the presence
6 of certain patterns of feature evolution and loss, and using temporal branch lengths for PD
7 in settings that may not be appropriate (e.g. due to rapid evolution of certain features over
8 short periods of time). Our paper also explores the relationship between the ‘Fair
9 Proportion’ index of PD and a simple index of FD (both of which correspond to Shapley
10 values in cooperative game theory). In a second mathematical result, we show that the two
11 indices can take identical values for any phylogenetic tree, provided the branch lengths in
12 the tree are chosen appropriately.

13 *Key words:* Phylogenetic diversity, feature diversity, evolutionary distinctiveness, Shapley
14 value

INTRODUCTION

Almost 30 years ago, Dan Faith published a seminal paper that laid out how phylogenies might aid in identifying sets of species with maximal “feature diversity” (Faith, 1992). Faith’s stated goal was to support practical biodiversity conservation in the face of limited resources, coupled with the assumption that maximising feature diversity (the total number of unique character states represented by a set of taxa) was a desirable conservation target.

Drawing on the call of Vane-Wright et al. (1991) to consider taxonomic distinctiveness when prioritizing species, Faith introduced the phylogenetic diversity (PD) metric, simply the sum of the edge lengths of the minimal subtree linking a subset of species to the root of the encompassing phylogeny (also called the ‘minimum spanning path’ by Faith (1992)). Importantly, these edge lengths were given in units of reconstructed character changes under maximum parsimony on the cladogram representing a character state matrix with no homoplasy. Faith showed, with an example, that the sum of these reconstructed edge lengths would lead to the same total feature diversity as that calculated from the character matrix itself. Importantly, if these cladistic edge lengths are representative of all features, then maximising PD (e.g. over a given subset size) would maximise feature diversity, even in the face of some homoplasy. The bulk of Faith’s 1992 paper was devoted to introducing the machinery to maximise PD.

Efficient algorithms for finding maximum PD sets are available (Bordewich et al. (2008)), the metric has been extended to networks (Minh et al. (2009)), and there are countless case studies that both measure and optimize PD for conservation (see, e.g., Pollock et al. (2017)); Faith’s original paper has been cited in excess of 2000 times. A recent review (Tucker et al., 2019) considered the literature concerning both the empirical correlations between PD and feature diversity, and the expected relationship between PD

41 and various conservation values.

42 Surprisingly, though, the necessary conditions under which PD will capture feature
43 diversity have never been formalized. Here, by using discrete characters, a model with no
44 homoplasy, and appropriate edge lengths, we prove that the PD of a subtree does indeed
45 measure feature diversity as defined by (Faith, 1992). This proof allows us to state more
46 formally when PD does not necessarily capture feature diversity, thereby allowing for
47 further modelling and statistical evaluation of the expected relationship under more
48 realistic models. Given the close connection between PD and taxonomic distinctiveness, we
49 also consider the conditions under which its phylogenetic measure (specifically the Shapley
50 value of evolutionary isolation) can capture its feature-based analogue.

51 PRELIMINARIES

52 *Feature diversity*

53 Consider a set X of taxa with $|X| = n$, and suppose that each taxon $x \in X$ has an
54 associated finite set F_x of ‘features’. To allow extra generality, we will assume that each
55 element $f \in F_x$ has a corresponding positive score $\mu(f) \in \mathbb{R}^{>0}$, which might be viewed as a
56 measure of the complexity, novelty, or richness of f (the default option is to set $\mu(f) = 1$
57 for all f). Let \mathcal{F} denote the set of all features present amongst the taxa in the collection
58 X , and let $\mathbb{F} = (F_x : x \in X)$ be the ordered n -tuple containing the feature sets of the taxa
59 in X . We will sometimes call \mathbb{F} a *feature assignment* as it summarizes how a set of features
60 is assigned to each taxon in X .

61 Note that \mathbb{F} provides the same information as a table showing the presence and
62 absence of features across taxa. So if $X = \{a, b, c\}$, then the feature assignment
63 $\mathbb{F} = (F_a, F_b, F_c)$ where $F_a = \{f_1, f_2\}$, $F_b = \{f_1, f_3\}$ and $F_c = \{f_2, f_3\}$, corresponds to a
64 standard character state matrix where there are two states per feature: presence (1) or
65 absence (0) (see Table 1).

Table 1. A standard character state matrix (0 = absence, 1 = presence) representing the assignment of three features (f_1, f_2, f_3) across three taxa (a, b, c).

Taxon	f_1	f_2	f_3
a	1	1	0
b	1	0	1
c	0	1	1

Given a subset Y of X , let

$$\nu_{\mathbb{F}}(Y) := \sum_{f \in \cup_{x \in Y} F_x} \mu(f).$$

Thus, $\nu_{\mathbb{F}}(Y)$ is the sum of the values of the features that are present in at least one taxon in Y . We refer to $\nu_{\mathbb{F}}(Y)$ as the *feature diversity* (FD) of Y . Note that in this sum, each feature is counted only once if present.

The function $\nu_{\mathbb{F}}$ (which assigns each subset Y of X a non-negative real value $\nu_{\mathbb{F}}(Y)$) clearly satisfies the following two properties: $\nu_{\mathbb{F}}(\emptyset) = 0$ and $\nu_{\mathbb{F}}$ is monotone (i.e. $Y \subseteq Y' \Rightarrow \nu_{\mathbb{F}}(Y) \leq \nu_{\mathbb{F}}(Y')$). Moreover, $\nu_{\mathbb{F}}$ also satisfies the submodularity inequality:

$$\nu_{\mathbb{F}}(Y \cup Y') + \nu_{\mathbb{F}}(Y \cap Y') \leq \nu_{\mathbb{F}}(Y) + \nu_{\mathbb{F}}(Y'), \quad (1)$$

and a proof is provided in the ‘Proofs of Propositions’ section.

Phylogenetic diversity

Now consider a rooted phylogenetic X -tree $T = (V, E)$ with root ρ , leaf set X , and edge length assignment $\ell : E \rightarrow \mathbb{R}^{\geq 0}$. For technical reasons (by allowing greater generality in the statement of our results) we assume that T has an additional ‘stem edge’ (ρ', ρ) where ρ' is a degree-1 vertex and ρ has in-degree 1 and out-degree at least 2 (see Fig. 1). The *phylogenetic diversity* (PD) of a subset Y of X is usually defined as the sum of the lengths of the edges in the minimal subtree of T that contains the leaves in Y and the root ρ of T . Here, we extend this definition by also including the length of the stem edge (ρ', ρ) in the calculation of PD for any subset $Y \subseteq X$ with $|Y| \geq 1$. This adds a constant, namely $\ell((\rho', \rho))$, to all subsets $Y \subseteq X \setminus \emptyset$ but does not affect properties of PD, such as its

83 monotonicity or submodularity.

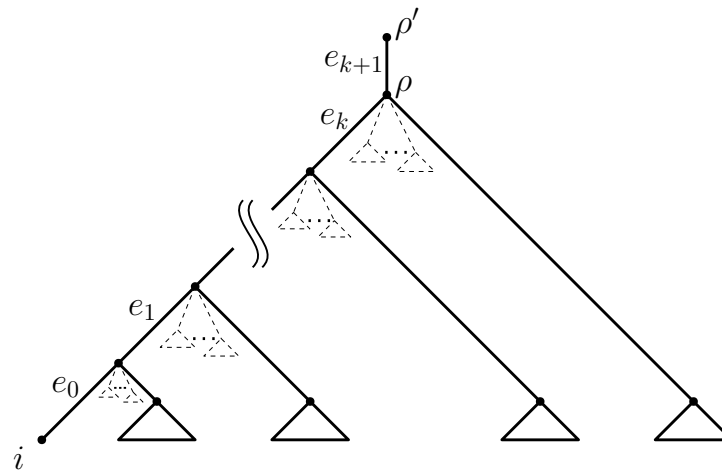


Fig. 1. Representing a phylogenetic X -tree T relative to a reference leaf i . Note that T is not assumed to be binary.

84 LINKING FEATURE DIVERSITY TO PHYLOGENETIC DIVERSITY

85 Next consider a model, based on a rooted phylogenetic X -tree T in which (i) each
 86 feature in \mathcal{F} arises on exactly one edge of T and (ii) each feature that arises is never lost
 87 and is passed down to all descendant vertices (including the leaves). This is just a model
 88 where every feature is a perfect synapomorphy.

89 We can describe this more precisely by specifying a map $h : \mathcal{F} \rightarrow E$, which indicates
 90 which edge each given feature arises on (note that several features may arise on the same
 91 edge). Thus $h^{-1}(e)$ denotes the set of features that arise on edge e . Here, we assume that
 92 $h^{-1}(e) \neq \emptyset$ for all interior edges of T (i.e., each interior edge of T gives rise to at least one
 93 feature). Notice that this is equivalent to allowing interior edges with ‘no event’ (i.e.,
 94 without a feature arising on them) and then contracting all interior ‘no event’ edges.

95 Note, however, that there may be pendant edges incident to leaves of T , on which
 96 no features arise. Furthermore, we also consider the stem edge (ρ', ρ) of T to be a pendant
 97 edge; in particular, no features arise on this stem edge precisely when there is no feature
 98 that is present in every taxon.

99 Under this model, F_x is then equal to the union of the sets $h^{-1}(e)$ over all the edges

100 e on the (unique) path from ρ' to leaf x .

101 When a feature assignment \mathbb{F} can be realized in this way, we will denote this by
102 writing $\mathbb{F} = F[T, h]$. Not every feature assignment \mathbb{F} can be realized in this way (on any
103 tree). As an example, consider the feature assignment described by the character state
104 matrix above (Table 1). In this case, there is no rooted phylogenetic X -tree $T = (V, E)$
105 and map $h : \{f_1, f_2, f_3\} \rightarrow E$ for which $(F_a, F_b, F_c) = F[T, h]$.

106 Fortunately, it is easy to characterise precisely when a feature assignment \mathbb{F} can be
107 realized as $F[T, h]$, and where T is either stipulated or not. The required condition
108 corresponds to the well-known structure of characters necessary (and sufficient) to
109 perfectly fit a common phylogenetic tree, namely that character states are arranged among
110 taxa as a set of nested apomorphies.

111 To describe this, we first introduce some additional notation. Let
112 $X_f := \{x \in X : f \in F_x\}$ denote the subset of taxa in X that have feature f . Moreover, let
113 $\mathcal{C}_{\mathcal{F}} := \{X_f : f \in \mathcal{F}\}$ be the collection of the sets X_f . The following result easily follows
114 from other well-known results in phylogenetics; however, for completeness a self-contained
115 proof is given in the ‘Proofs of Propositions’ section.

116 **Proposition 1**

117 (i) $\mathbb{F} = F[T, h]$ for some $h : \mathcal{F} \rightarrow E$ if and only if X_f corresponds to a cluster of T for
118 each feature $f \in \mathcal{F}$. Moreover, when $\mathbb{F} = F[T, h]$, the map h is uniquely determined:
119 for each $f \in \mathcal{F}$, $h(f)$ is the edge directly above the most recent common ancestor of
120 the taxa in X_f .

121 (ii) There exists a tree T and map h such that $\mathbb{F} = F[T, h]$ if and only if $\mathcal{C}_{\mathcal{F}}$ is a
122 hierarchy on X . In other words, for all pairs $X_f, X_{f'} \in \mathcal{C}_{\mathcal{F}}$, we have
123 $X_f \cap X_{f'} \in \{\emptyset, X_f, X_{f'}\}$ (i.e. X_f and $X_{f'}$ are either disjoint or nested).

124

FIRST MAIN RESULT

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We can now describe the relationship between FD and PD in a precise way.

126

Theorem 1 Let T be a rooted phylogenetic X -tree and let \mathbb{F} be an assignment of features across the taxa in X .

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(i) $\mathbb{F} = F[T, h]$ for some function $h : \mathcal{F} \rightarrow E$ if and only if $\nu_{\mathbb{F}}$ is exactly equal to the PD function for some edge length assignment ℓ of T that assigns strictly positive lengths to all interior edges of T and non-negative lengths to all pendant edges and the stem edge (ρ', ρ) (i.e. $\nu_{\mathbb{F}}(Y) = PD_{(T, \ell)}(Y)$ for all subsets Y of X).

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(ii) When (i) holds, h and ℓ are both uniquely determined. In particular, $\ell = \ell_h$, where, for each $f \in \mathcal{F}$, $\ell_h(e) := \sum_{f: h(f)=e} \mu(f)$ (and $\ell_h(e) = 0$ for each pendant edge e of T with $h^{-1}(e) = \emptyset$).

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Proof of Theorem 1.

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The proof of Theorem 1 relies on three lemmas (whose proof is given in the

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Appendix). We state these lemmas now, and then use them to establish Theorem 1.

Lemma 1 Given a rooted phylogenetic X -tree T , suppose that $\mathbb{F} = F[T, h]$ for some map $h : \mathcal{F} \rightarrow E$. Let $\ell_h : E \rightarrow \mathbb{R}^{\geq 0}$ be defined by setting

$$\ell_h(e) := \sum_{f: h(f)=e} \mu(f),$$

for each edge e of T (where $\ell_h(e) := 0$ if $h^{-1}(e) = \emptyset$). Then, for all subsets Y of X we have:

$$\nu_{\mathbb{F}}(Y) = PD_{(T, \ell_h)}(Y).$$

Lemma 2 Given a rooted phylogenetic X -tree T , suppose that the identity

$$\nu_{\mathbb{F}}(Y) = PD_{(T, \ell)}(Y)$$

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holds for all subsets $Y \subseteq X$, where $\ell : E \rightarrow \mathbb{R}^{\geq 0}$ is such that the interior edges of T are

139 assigned strictly positive lengths and pendant edges (including the stem edge) are assigned
140 non-negative lengths. Then, there exists a map $h : \mathcal{F} \rightarrow E$ such that $\mathbb{F} = F[T, h]$.

141 **Lemma 3** Let T be a rooted phylogenetic X -tree (with additional stem edge). Then, the
142 edge lengths of T are uniquely determined by the induced PD scores of all subsets $Y \subseteq X$
143 with $|Y| \leq 2$.

We now show that Theorem 1 follows from these lemmas. Part (i) of Theorem 1,
namely

$$\mathbb{F} = F[T, h] \Leftrightarrow \nu_{\mathbb{F}}(Y) = PD_{(T, \ell)}(Y) \forall Y \subseteq X$$

144 follows from Lemmas 1 and 2 (the ‘only if’ implication is implied by Lemma 1 and the ‘if’
145 implication is implied by Lemma 2).

146 For Part (ii), the uniqueness of ℓ (i.e., $\ell = \ell_h$), follows by combining Lemmas 1 and
147 3. More precisely, Lemma 1 states that assigning edge lengths according to ℓ_h induces the
148 equality of $\nu_{\mathbb{F}}(Y)$ and $PD_{(T, \ell_h)}(Y)$ for all $Y \subseteq X$, whereas, by Lemma 3, the edge lengths
149 of a given tree T are uniquely determined by the induced PD scores of all $Y \subseteq X$ (indeed,
150 even those with size at most 2 suffice). Moreover, the uniqueness of h is implied by
151 Proposition 1, Part (i). This completes the proof. \square

152 DIVERSITY INDICES

153 A *diversity index* for FD (or PD) is a score assigned to each taxon $x \in X$ that sums
154 to the total FD (or PD, respectively) of X . Diversity indices can be viewed as a way to
155 apportion FD (or PD) fairly among the extant taxa. Although there are various ways to do
156 this, we focus on one that is characterised by simple axioms, namely, the Shapley value
157 (from cooperative game theory), which coincides, in the PD setting, with the well-known
158 Fair Proportion index (described below).

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Feature diversity index

Given \mathbb{F} , let

$$\varphi_{\mathbb{F}} : X \rightarrow \mathbb{R}^{\geq 0}$$

be the function defined by:

$$\varphi_{\mathbb{F}}(x) := \sum_{f \in F_x} \frac{\mu(f)}{n(f)},$$

160 where $n(f)$ is the number of taxa that have feature f (i.e. $n(f) = |X_f|$). In words, $\varphi_{\mathbb{F}}(x)$
161 assigns to each taxon x a sum of scores — one score for each of its features — where the
162 score for feature f is $\mu(f)$ if x is the only taxon having this feature; otherwise, the score
163 equals $\mu(f)$ divided by the total number of taxa having feature f .

164 The following result provides a formal justification for regarding $\varphi_{\mathbb{F}}$ as a natural
165 index of FD. Note that this index does not depend on any underlying phylogeny, or on
166 assumptions concerning feature evolution, and is easily computed.

167 The result is phrased within the general framework of cooperative game theory (a
168 topic more well-known in economics than biology, though it has recently been applied to
169 PD, as we discuss below). In this general framework, one has a finite set X and a function
170 s that assigns to each subset Y of X a corresponding score $s(Y)$ with $s(\emptyset) = 0$ (in our
171 current setting $s(Y) = \nu_{\mathbb{F}}(Y)$). Given the pair (X, s) , one seeks to apportion the score of
172 the full set X among each of its elements according to an index (i.e., a value for each
173 element of X) in a way that reflects the contribution each element makes to the total
174 score. In this general framework, there is a particular index, called the *Shapley value*, that
175 is uniquely determined by well-motivated axioms, and which is given by an explicit (if
176 somewhat complex) combinatorial expression (Shapley, 1953).

177 **Proposition 2** The FD index $\varphi_{\mathbb{F}}$ is precisely the Shapley value for the pair $(X, \nu_{\mathbb{F}})$. In
178 particular, $\sum_{x \in X} \varphi_{\mathbb{F}}(x) = \nu_{\mathbb{F}}(X)$.

179 The proof of Proposition 2 is provided in the ‘Proofs of Propositions’ section.

Phylogenetic diversity index

Given the pair (T, ℓ) , the *Fair Proportion index* (FP) (from Redding (2003) and Redding et al. (2007), see also Isaac et al. (2007)) for taxon x is given by:

$$FP_{(T,\ell)}(x) = \sum_{e \in P(T; \rho', x)} \frac{1}{n(e)} \cdot \ell(e),$$

where $P(T; \rho', x)$ denotes the unique path from ρ' to x and where $n(e)$ is the number of leaves descending from the endpoint of edge e closest to the leaves.

It turns out that the FP index coincides exactly with the Shapley value based on PD (i.e. when PD is used as the characteristic function in the underlying cooperative game), a result first shown by Fuchs and Jin (2015). As $\varphi_{\mathbb{F}}$ is (by Proposition 2) equivalent to the Shapley value based on FD, Theorem 1 thus has the interesting implication that if a feature assignment \mathbb{F} can be realized on a tree (i.e., if $\mathbb{F} = F[T, h]$), then the Shapley values based on PD and FD coincide.

Proposition 3 If $\mathbb{F} = F[T, h]$, then $\varphi_{\mathbb{F}}(x)$ is equal to the Fair Proportion index for taxon x on tree T for the edge length assignment ℓ_h .

Proof. Let $\mathbb{F} = F[T, h]$ and let $x \in X$. As noted above, we have:

$$FP_{(T,\ell_h)}(x) = \sum_{e \in P(T; \rho', x)} \frac{1}{n(e)} \cdot \ell_h(e).$$

Importantly, we can also write $\varphi_{\mathbb{F}}(x)$ as follows:

$$\varphi_{\mathbb{F}}(x) = \sum_{f \in F_x} \frac{\mu(f)}{n(f)} = \sum_{\substack{e \in E(T): \\ \exists f \in F_x \text{ with } h(f)=e}} \frac{\ell_h(e)}{n(f)}.$$

Now, since $\mathbb{F} = F[T, h]$, all the edges on which features present in F_x arise must lie on the unique path from ρ' to x . Moreover, a feature f' not contained in F_x , cannot have arisen on this path. More precisely, if a feature f arises on edge e , then a taxon $x \in X$ has this feature if and only if it is a descendant of e . In particular, $n(f) = n(e)$. In summary, this implies that $\varphi_{\mathbb{F}}(x) = FP_{(T,\ell_h)}(x)$. □

196 We now establish a further result. We show that $\varphi_{\mathbb{F}}(x)$ can always be interpreted as
197 $FP_{(T,\ell)}(x)$ for any tree T (even if $\mathbb{F} \neq F[T', h]$ for any tree T').

198 **Theorem 2** Let \mathbb{F} be a feature assignment such that $F_x \neq \emptyset$ for all $x \in X$, and let T be any
199 rooted phylogenetic X -tree (with additional stem edge). Then, there exists an edge length
200 assignment $\ell : E \rightarrow \mathbb{R}^{>0}$ that assigns strictly positive lengths to all edges of T , such that
201 $\varphi_{\mathbb{F}}(x) = FP_{(T,\ell)}(x)$ for all $x \in X$.

202 The proof of Theorem 2 is provided in the Appendix, however we provide an outline
203 of the argument here. First observe that if T is a star tree then Theorem 2 clearly holds,
204 since we can simply assign edge length $\varphi_{\mathbb{F}}(x)$ to the edge incident with leaf x and obtain
205 $\varphi_{\mathbb{F}}(x) = FP_{(T,\ell)}(x)$ for all $x \in X$. If T is not a star tree, then we could assign edge length 0
206 to all the interior edges and the stem edge, and apply the same trick to obtain the required
207 identity. The non-trivial part of the proof of Theorem 2 is to show that one can ‘lift’ some
208 fraction of the lengths of the pendant edges so as that (i) *all* edges of T have strictly
209 positive length, and in such a way that (ii) the required identity between the FD and PD
210 diversity indices holds for each taxon x .

211 DISCUSSION

212 It would be a mistake to interpret Theorem 1 above as stating that feature diversity
213 coincides with phylogenetic diversity (on a given tree with suitably chosen branch lengths)
214 only under evolutionary scenarios in which features arise once in the tree and are never
215 lost. Instead, Theorem 1 states that these two measures coincide precisely when the
216 distribution of features across taxa can be described by such a single-gain-and-no-loss
217 model, even if the underlying reality might be different. For instance, a feature can arise
218 along a stem edge, be lost in one of the two descendant edges, but arise again in its
219 descendants such that the entire crown clade expresses the feature. The feature’s true
220 history is obscured but its distribution is still perfectly congruent with the underlying tree

221 and thus meets the conditions of Proposition 1.

222 This points to one scenario where Theorem 1 will not hold, where the rate of
223 evolution is high enough and the state space is small enough (e.g., features are discrete and
224 can be both gained and lost) that at least some features have non-trivial probabilities of
225 arising more than once on a tree. Faith (1992) astutely pointed out that such convergent
226 features “are not predictive of similarities of other features,” such that “greater
227 phylogenetic diversity will, on average, imply greater feature diversity as defined by any
228 particular collection of features.” Because empirical measures of PD and measured FD
229 need not coincide (Devictor et al. (2010); see also the discussion in Winter et al. (2013)),
230 one critical question is whether there are subsets of features that simultaneously (i) are
231 more valuable to conservation than the average feature and (ii) are (or are likely to be)
232 convergent, perhaps due to parallel adaptation (Mazel et al. (2018, 2019); Owen et al.
233 (2019)). To the extent that there are, the force of Faith’s all-important “average” PD = FD
234 statement weakens. However, answering the question is non-trivial because it requires that
235 we know about the mode of evolution of conservation-relevant features in a focal clade. The
236 only attempt to test this we know of is by Forest et al. (2007) for Southern African plants,
237 where the patterns supported Faith’s average argument. More tests would be welcome.

238 A second (related) reason why Theorem 1 allows PD and FD to diverge in
239 applications is that even when $\mathbb{F} = F[T, h]$, the edge lengths must be suitably chosen.
240 Under a stochastic process in which features arise independently at a constant (and very
241 small) rate r , then conditional on a feature arising (at least) once in the tree, as $r \rightarrow 0$, the
242 expected number of features that arise on an edge will be proportional to the temporal
243 length of that edge (and each trait will arise exactly once in the tree). This (coupled with
244 Faith’s “average” argument) is the justification for using time-calibrated ultrametric
245 phylogenetic trees when comparing PD scores. However, the evolution of some important
246 subset of features may not be captured with this model at all (Mazel et al. (2017)), or,
247 more prosaically, may simply evolve at such a high rate that the time-calibrated

248 ultrametric tree edge lengths are not predictive of the number and placement of features
249 (for example, due to saturation). Here again, both theoretical (see e.g. Tucker et al.
250 (2018)) and empirical tests using features of known conservation value are needed.

251 Two observations can be made on the basis of Theorem 2. The first is that the
252 compact expression for the $\varphi_{\mathbb{F}}(x)$ measure of feature diversity does not require any
253 particular model of feature evolution on a tree: different features and different subtrees can
254 be governed by different processes. While we might still require Faith (1992)’s “average”
255 argument, namely, that the distribution of measured features mirrors the features of
256 conservation concern more generally, this might expand its usefulness. Once again, this is
257 open to empirical testing. However, the Shapley value is quite specific in what it measures:
258 it is the expected contribution (here, of features) to all possible future subsets of taxa,
259 where subset sizes are equiprobable (Steel, 2016). This is a strong assumption that bears
260 further scrutiny (see also Faith (2008)).

261 In conclusion, our paper provides a precise mathematical framework to help address
262 some fundamental questions and possible future approaches concerning the link between
263 feature and phylogenetic diversity, a critical connection for phylogeny-oriented
264 conservation triage.

265 PROOFS OF PROPOSITIONS

266 *Proof of Proposition 1.*

267 (i) First, suppose that $\mathbb{F} = F[T, h]$, and let $f \in \mathcal{F}$ be an arbitrary feature. Moreover, let
268 $e = h(f)$ be the edge f arose on. Then, precisely those leaves of T that are
269 descendants of e contain feature f . In particular, X_f corresponds to a cluster of T
270 (namely, to the cluster of leaves descending from e).

271 Now, suppose that X_f corresponds to a cluster of T for each feature $f \in \mathcal{F}$. Then we
272 can realize \mathbb{F} on T by setting $h(f)$ to the edge directly above the most recent

273 common ancestor of the taxa in X_f for each $f \in \mathcal{F}$. In particular, $\mathbb{F} = F[T, h]$.

274 Moreover, when $\mathbb{F} = F[T, h]$, $h(f)$ must be the edge, say e , directly above the most
 275 recent common ancestor of the taxa in X_f . If f had arisen above e , say on some edge
 276 e' , there would be at least one taxon x in the cluster $c_T(e')$ induced by e' (i.e. in the
 277 set of leaves of T that are separated from the root of T by e') with $x \in c_T(e') \setminus X_f$.

278 This, however, would imply that f was lost on the way from e' to x , which is a
 279 contradiction. Similarly, if f had arisen below edge e , say on some edge e'' , this
 280 would imply that the cluster $c_T(e'')$ induced by e'' was a strict subset of X_f , i.e.
 281 $c_T(e'') \subset X_f$. In other words, there would be at least one taxon $y \in X_f \setminus c_T(e'')$,
 282 which implies that f arose at least twice in T . This is again a contradiction.

283 (ii) First, suppose that $\mathbb{F} = F[T, h]$. By Part (i) of this Lemma, this implies that the set
 284 X_f corresponds to a cluster of T for all $f \in \mathcal{F}$. In particular, $\mathcal{C}_{\mathcal{F}} = \{X_f : f \in \mathcal{F}\}$ is a
 285 set of clusters induced by a rooted phylogenetic X -tree T , which implies that $\mathcal{C}_{\mathcal{F}}$ is a
 286 hierarchy on X (cf. Proposition 2.1 in Steel (2016)).

287 Now, suppose that $\mathcal{C}_{\mathcal{F}}$ is a hierarchy on X . This implies (again by Proposition 2.1 in
 288 Steel (2016)) that $\mathcal{C}_{\mathcal{F}}$ is the set of clusters of some rooted phylogenetic X -tree T . By
 289 Part (i) of this Lemma, this in turn implies that $\mathbb{F} = F[T, h]$.

290 □

Proof of Proposition 2: Notice that both $\varphi_{\mathbb{F}}(x)$ and $\nu_{\mathbb{F}}(Y)$ (with $Y \subseteq X$) are linear functions in $\mu(f)$. More precisely,

$$\varphi_{\mathbb{F}}(x) = \sum_{f \in \mathcal{F}} \gamma(x, f) \cdot \mu(f), \quad \text{where} \quad \gamma(x, f) = \begin{cases} \frac{1}{n(f)}, & \text{if } f \in F_x; \\ 0, & \text{otherwise.} \end{cases}$$

Analogously,

$$\nu_{\mathbb{F}}(Y) = \sum_{f \in \mathcal{F}} \gamma'(Y, f) \cdot \mu(f), \quad \text{where} \quad \gamma'(Y, f) = \begin{cases} 1, & \text{if } f \in \cup_{x \in Y} F_x; \\ 0, & \text{otherwise.} \end{cases}$$

291 Thus, by linearity (see also Lemma 6.14 in Steel (2016)), it suffices to show the statements
 292 for the case that one element of \mathcal{F} , say f_i , has score $\mu(f_i) = 1$, whereas $\mu(f_j) = 0$ for all

293 $f_j \in \mathcal{F} \setminus \{f_i\}$ (note that μ was earlier defined to be strictly positive, but we are here
 294 relaxing this for algebraic convenience).

295 For the first part of the proof, recall that given the cooperative game $(X, \nu_{\mathbb{F}})$, the
 296 Shapley value of $x \in X$ is defined as (Shapley (1953))

$$SV_{\nu_{\mathbb{F}}}(x) = \frac{1}{n!} \sum_{S \subseteq X: x \in S} (|S| - 1)! (n - |S|)! \Delta(S, x), \quad (2)$$

297 where $\Delta(S, x) = \nu_{\mathbb{F}}(S) - \nu_{\mathbb{F}}(S \setminus \{x\})$. We now show that $SV_{\nu_{\mathbb{F}}}(x) = \varphi_{\mathbb{F}}(x)$ (where we
 298 assume that $\mu(f_i) = 1$ and $\mu(f_j) = 0$ for all $f_j \in \mathcal{F} \setminus \{f_i\}$).

299 We can distinguish two cases:

- 300 • If $f_i \notin F_x$, then $\Delta(S, x) = 0$ for all S , and thus, $SV_{\nu_{\mathbb{F}}}(x) = 0$. On the other hand, we
 301 clearly also have $\varphi_{\mathbb{F}}(x) = 0$.
- If $f_i \in F_x$, then $\Delta(S, x) = 1$ if (i) $x \in S$ and (ii) there is no $y \in S$ with $f_i \in F_y$;
 otherwise $\Delta(S, x) = 0$. Let $C \subseteq X$ be the set of taxa that have feature f_i , i.e.,
 $C = \{y \in X : f_i \in F_y\}$, and so $n(f_i) = |C|$. Then, $SV_{\nu_{\mathbb{F}}}$ can be written as

$$\begin{aligned} & \frac{1}{n!} \sum_{\substack{S: x \in S \\ S \setminus \{x\} \subseteq X \setminus C}} (|S| - 1)! (n - |S|)! \cdot 1 \\ &= \frac{1}{n!} \sum_{k=1}^{n-n(f_i)+1} \binom{n - n(f_i)}{k - 1} (k - 1)! (n - k)! = \frac{1}{n(f_i)}, \end{aligned}$$

302 where the last equality follows from the fact that $\frac{1}{n!} \sum_{j=0}^{n-r} \binom{n-r}{j} j! (n - 1 - j)! = \frac{1}{r}$ for
 303 $1 \leq r \leq n$ (Lemma 6.15 in Steel (2016)) (here: $j = k - 1$ and $r = n(f_i)$). On the
 304 other hand, $\varphi_{\mathbb{F}}(x) = \frac{\mu(f_i)}{n(f_i)} = \frac{1}{n(f_i)}$, which completes the proof.

The second part of Proposition 2, follows directly from properties of the Shapley value; however we give a direct proof. Again, it suffices to consider the case where $\mu(f_i) = 1$ and $\mu(f_j) = 0$, for all $j \neq i$, in which case we obtain the required equality:

$$\sum_{x \in X} \varphi_{\mathbb{F}}(x) = \sum_{\substack{x \in X: \\ f_i \in F_x}} \varphi_{\mathbb{F}}(x) + \sum_{\substack{x \in X: \\ f_i \notin F_x}} \varphi_{\mathbb{F}}(x) = \sum_{\substack{x \in X: \\ f_i \in F_x}} \frac{\mu(f_i)}{n(f_i)} + 0 = \mu(f_i) = 1 = \nu_{\mathbb{F}}(X).$$

Proof of Inequality (1). Let $W(Y) := \bigcup_{x \in Y} F_x$. From the proof of Proposition 2 we have:

$$\nu_{\mathbb{F}}(Y) = \sum_{f \in \mathcal{F}} \gamma'(Y, f) \cdot \mu(f), \quad \text{where} \quad \gamma'(Y, f) = \begin{cases} 1, & \text{if } f \in W(Y); \\ 0, & \text{otherwise.} \end{cases}$$

Now,

$$W(Y \cup Y') = W(Y) \cup W(Y'),$$

and

$$W(Y \cap Y') \subseteq W(Y) \cap W(Y'),$$

(and the containment can be strict). It follows that for all $f \in \mathcal{F}$ and all $Y, Y' \subseteq X$:

$$\gamma'(Y \cup Y', f) + \gamma'(Y \cap Y', f) - \gamma'(Y, f) - \gamma'(Y', f) \leq 0.$$

306 Since $\nu_{\mathbb{F}}(Y \cup Y') + \nu_{\mathbb{F}}(Y \cap Y') - \nu_{\mathbb{F}}(Y) - \nu_{\mathbb{F}}(Y')$ is a positive weighted sum of the
307 corresponding γ' quantities above, Inequality (1) now follows.

ACKNOWLEDGEMENTS

310 MS thanks the Royal Society of NZ (Catalyst Grant) for funding support. AOM is
311 supported by the Natural Sciences and Engineering Research Council of Canada, and is
312 grateful to members of the iDiv synthesis centre working group “Conservation and
313 Phylogenies” for ongoing discussion, and Dan Faith for continual engagement on this topic.

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APPENDIX: PROOF OF LEMMAS 1–3, AND THEOREM 2.

Proof of Lemma 1. Suppose that $\mathbb{F} = F[T, h]$. For each $f \in \mathcal{F}$, let X_f be the set of taxa that have feature f . Then,

$$\nu_{\mathbb{F}}(Y) = \sum_{\substack{f \in \mathcal{F}: \\ X_f \cap Y \neq \emptyset}} \mu(f) = \sum_{\substack{e \in E(T): \\ \exists f \in \mathcal{F}: h(f) = e \text{ and } X_f \cap Y \neq \emptyset}} \ell_h(e), \quad (3)$$

where the last equality follows from the fact that $\mathbb{F} = F[T, h]$.

On the other hand,

$$PD_{(T, \ell_h)}(Y) = \sum_{\substack{e \in E(T): \\ c_T(e) \cap Y \neq \emptyset}} \ell_h(e), \quad (4)$$

where $c_T(e)$ denotes the set of leaves of T that are separated from the root of T by e . Now, as $\mathbb{F} = F[T, h]$, when $e = h(f)$, $c_T(e)$ corresponds to the set X_f . Thus, for $e \in E(T)$, we can conclude that $c_T(e) \cap Y \neq \emptyset$ precisely if

- $\exists f \in \mathcal{F} : h(f) = e$ and $X_f \cap Y \neq \emptyset$, or
- $\nexists f \in \mathcal{F} : h(f) = e$ and e is a pendant edge incident to a leaf $y \in Y$ (in which case $\ell_h(e) = 0$).

Thus, we can re-write Eqn. (4) as

$$PD_{(T, \ell_h)}(Y) = \sum_{\substack{e \in E(T): \\ \exists f \in \mathcal{F}: h(f) = e \text{ and } X_f \cap Y \neq \emptyset}} \ell_h(e) = \nu_{\mathbb{F}}(Y),$$

where the last equality follows from Eqn. (3). This completes the proof. \square

Proof of Lemma 2:. We will prove this statement by contradiction. Thus, assume that $\nu_{\mathbb{F}}(Y) = PD_{(T, \ell)}(Y)$ for all $Y \subseteq X$ but there is no map $h : \mathcal{F} \rightarrow E$ such that $\mathbb{F} = F[T, h]$. We now distinguish two cases: (i) \mathbb{F} cannot be explained by T , but by some other tree T' , i.e. $\mathbb{F} = F[T', h']$, or (ii) the collection of sets $\mathcal{C}_{\mathcal{F}} = \{X_f : f \in \mathcal{F}\}$ does not form a hierarchy and cannot be explained by any tree (cf. Proposition 1, Part (ii)).

(i) First, suppose that $\mathbb{F} \neq F[T, h]$ but $\mathbb{F} = F[T', h']$, and $\nu_{\mathbb{F}}(Y) = PD_{(T, \ell)}(Y)$ for all

389 $Y \subseteq X$. Now, as $T \neq T'$, there must be some $i, j, k \in X$ such that restricting T and
 390 T' to $\{i, j, k\}$ yields distinct trees. More precisely, there exist $i, j, k \in X$ such that

- 391 (a) $T|_{\{i,j,k\}}$ is either the caterpillar tree on three leaves with cherry $[i, j]$ or the
 392 rooted star tree on $\{i, j, k\}$,
- 393 (b) $T'|_{\{i,j,k\}}$ is either the caterpillar tree on three leaves with cherry $[i, k]$ or the
 394 rooted star tree on $\{i, j, k\}$,
- 395 (c) $T|_{\{i,j,k\}} \neq T'|_{\{i,j,k\}}$ (in particular, $T|_{\{i,j,k\}}$ and $T'|_{\{i,j,k\}}$ are not both star trees).

396 Let $\Delta_{\mathbb{F}}(x, x') := \nu_{\mathbb{F}}(\{x\}) + \nu_{\mathbb{F}}(\{x'\}) - \nu_{\mathbb{F}}(\{x, x'\})$, for each distinct pair $x, x' \in X$.

397 Then as $\nu_{\mathbb{F}}(Y) = PD_{(T,\ell)}(Y)$ for all $Y \subseteq X$, we have from (a) that:

$$\Delta_{\mathbb{F}}(i, j) \begin{cases} = \Delta_{\mathbb{F}}(i, k), & \text{if } T|_{\{i,j,k\}} \text{ is a star tree;} \\ > \Delta_{\mathbb{F}}(i, k), & \text{otherwise.} \end{cases} \quad (5)$$

398 On the other hand, as $\mathbb{F} = F[T', h']$, we have by Lemma 1, that

399 $\nu_{\mathbb{F}}(Y) = PD_{(T', \ell_{h'})}(Y)$ for all $Y \subseteq X$ (where $\ell_{h'}(e) = \sum_{f: h'(f)=e} \mu(f)$; in particular,
 400 $\ell_{h'}(e) > 0$ for each interior edge e of T'). This implies that:

$$\Delta_{\mathbb{F}}(i, k) \begin{cases} = \Delta_{\mathbb{F}}(i, j), & \text{if } T'|_{\{i,j,k\}} \text{ is a star tree;} \\ > \Delta_{\mathbb{F}}(i, j), & \text{otherwise.} \end{cases} \quad (6)$$

401 Comparing Eqns. (5) and (6), and using the fact that $T|_{\{i,j,k\}}$ and $T'|_{\{i,j,k\}}$ cannot
 402 both be star trees, this yields a contradiction. As (i, j, k) was an arbitrary triple of
 403 leaves for which $T|_{\{i,j,k\}} \neq T'|_{\{i,j,k\}}$, this contradiction implies that the initial
 404 assumption was wrong. In particular, $\mathbb{F} = F[T, h]$.

405 (ii) Now, assume that $\nu_{\mathbb{F}}(Y) = PD_{(T,\ell)}(Y)$ for all $Y \subseteq X$, but $\mathcal{C}_{\mathcal{F}} = \{X_f : f \in \mathcal{F}\}$ does
 406 not form a hierarchy. This implies that there exists $f_1, f_2 \in \mathcal{F}$ such that

- 407 (a) There exists a taxon $x_1 \in X$ such that $x_1 \in X_{f_1} \cap X_{f_2}$.
- 408 (b) There exists a taxon $x_2 \in X$ such that $x_2 \in X_{f_1} \setminus X_{f_2}$.
- 409 (c) There exists a taxon $x_3 \in X$ such that $x_3 \in X_{f_2} \setminus X_{f_1}$.

We now partition the feature set \mathcal{F} into eight pairwise disjoint subsets A, \dots, G , where

$$A := \{f \in \mathcal{F} : f \in F_{x_1} \setminus (F_{x_2} \cup F_{x_3})\}$$

$$B := \{f \in \mathcal{F} : f \in F_{x_2} \setminus (F_{x_1} \cup F_{x_3})\}$$

$$C := \{f \in \mathcal{F} : f \in F_{x_3} \setminus (F_{x_1} \cup F_{x_2})\}$$

$$D := \{f \in \mathcal{F} : f \in (F_{x_1} \cap F_{x_2}) \setminus F_{x_3}\}$$

$$E := \{f \in \mathcal{F} : f \in (F_{x_1} \cap F_{x_3}) \setminus F_{x_2}\}$$

$$F := \{f \in \mathcal{F} : f \in (F_{x_2} \cap F_{x_3}) \setminus F_{x_1}\}$$

$$G := \{f \in \mathcal{F} : \bigcap_{i=1}^3 F_{x_i}\}$$

$$H := \{f \in \mathcal{F} : f \notin \bigcup_{i=1}^3 F_{x_i}\}$$

410 Note that $D \neq \emptyset$ (because by (a)–(c), $f_1 \in (F_{x_1} \cap F_{x_2}) \setminus F_{x_3}$). Analogously, $E \neq \emptyset$
 411 (because $f_2 \in (F_{x_1} \cap F_{x_3}) \setminus F_{x_2}$).

412 Given a set of features S , let $\mu(S) := \sum_{f \in S} \mu(f)$ denote the sum of scores of features
 413 present in S . As $\mu(f) > 0$ for all $f \in \mathcal{F}$, by the preceding argument, in particular
 414 $\mu(D), \mu(E) > 0$.

415 We now compute $\nu_{\mathbb{F}}(Y)$ for all $Y \subseteq \{x_1, x_2, x_3\}$ with $|Y| \geq 1$, and compare it to
 416 $PD_{(T, \ell)}(Y)$. Recall that $PD_{(T, \ell)}(Y)$ for $Y \subseteq X$ is computed by considering the sum of
 417 edge lengths in the minimum subtree of T connecting the taxa in Y and ρ' . Without
 418 loss of generality, we can assume that the subtree induced by $\{x_1, x_2, x_2\}$ has the
 419 structure depicted in Fig. 2 (otherwise, we exchange leaf labels).

Now, by assumption $\nu_{\mathbb{F}}(Y) = PD_{(T, \ell)}(Y)$ for all $Y \subseteq X$. For $Y \subseteq \{x_1, x_2, x_3\}$ with $|Y| \geq 1$, this gives rise to a system of 7 linear equations (where $\ell(p)$ denotes the

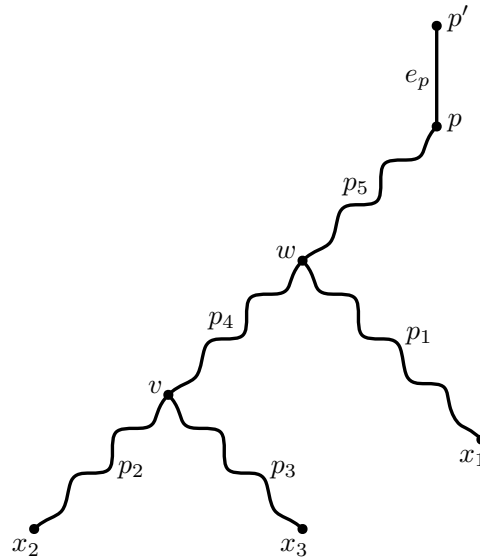


Fig. 2. Subtree induced by taxa x_1 , x_2 , and x_3 in the proof of Lemma 2. v denotes the most recent common ancestor of x_2 and x_3 . Analogously, w denotes the most recent common ancestor of x_1 , x_2 , and x_3 . Furthermore, p_1 denotes the unique path from w to x_1 , p_2 denotes the unique path from v to x_2 and so forth.

length of path p):

$$\nu_{\mathbb{F}}(\{x_1\}) = PD_{(T,\ell)}(\{x_1\})$$

$$\Leftrightarrow \mu(A) + \mu(D) + \mu(E) + \mu(G) = \ell(p_1) + \ell(p_5) + \ell(e_p)$$

$$\nu_{\mathbb{F}}(\{x_2\}) = PD_{(T,\ell)}(\{x_2\})$$

$$\Leftrightarrow \mu(B) + \mu(D) + \mu(F) + \mu(G) = \ell(p_2) + \ell(p_4) + \ell(p_5) + \ell(e_p)$$

$$\nu_{\mathbb{F}}(\{x_3\}) = PD_{(T,\ell)}(\{x_3\})$$

$$\Leftrightarrow \mu(C) + \mu(E) + \mu(F) + \mu(G) = \ell(p_3) + \ell(p_4) + \ell(p_5) + \ell(e_p)$$

$$\nu_{\mathbb{F}}(\{x_1, x_2\}) = PD_{(T,\ell)}(\{x_1, x_2\})$$

$$\Leftrightarrow \mu(A) + \mu(B) + \mu(D) + \mu(E) + \mu(F) + \mu(G) = \ell(p_1) + \ell(p_2) + \ell(p_4) + \ell(p_5) + \ell(e_p)$$

$$\nu_{\mathbb{F}}(\{x_1, x_3\}) = PD_{(T,\ell)}(\{x_1, x_3\})$$

$$\Leftrightarrow \mu(A) + \mu(C) + \mu(D) + \mu(E) + \mu(F) + \mu(G) = \ell(p_1) + \ell(p_3) + \ell(p_4) + \ell(p_5) + \ell(e_p)$$

$$\nu_{\mathbb{F}}(\{x_2, x_3\}) = PD_{(T,\ell)}(\{x_2, x_3\})$$

$$\Leftrightarrow \mu(B) + \mu(C) + \mu(D) + \mu(E) + \mu(F) + \mu(G) = \ell(p_2) + \ell(p_3) + \ell(p_4) + \ell(p_5) + \ell(e_p)$$

$$\nu_{\mathbb{F}}(\{x_1, x_2, x_3\}) = PD_{(T,\ell)}(\{x_1, x_2, x_3\})$$

$$\Leftrightarrow \mu(A) + \mu(B) + \mu(C) + \mu(D) + \mu(E) + \mu(F) + \mu(G)$$

$$= \ell(p_1) + \ell(p_2) + \ell(p_3) + \ell(p_4) + \ell(p_5) + \ell(e_p)$$

420 Solving this system of linear equations for $\mu(A), \dots, \mu(G)$ yields $\mu(A) = \ell(p_1)$,
 421 $\mu(B) = \ell(p_2)$, $\mu(C) = \ell(p_3)$, $\mu(D) = \mu(E) = 0$, $\mu(F) = \ell(p_4)$, and
 422 $\mu(G) = \ell(p_5) + \ell(e_\rho)$.

423 However, as our assumption implies that $\mu(D), \mu(E) > 0$, this is a contradiction.

424 Thus, the initial assumption was false. In particular, $\{X_f : f \in \mathcal{F}\}$ forms a hierarchy.

425 Thus, by Proposition 1, Part (ii), there exist T' and h' such that $\mathbb{F} = F[T', h']$. Now,
 426 by case (i) of this proof, this implies $\mathbb{F} = F[T, h]$. This completes the proof.

427 □

428 *Proof of Lemma 3:* Let T be a rooted phylogenetic X -tree (with additional stem edge),
 429 and assume that $PD_T(Y)$ is given for all $Y \subseteq X$ with $|Y| \leq 2$. We now show that we can
 430 uniquely infer the edge lengths of T from these scores. Let $i \in X$ be a leaf of T . Then,
 431 there is a unique path $e_{k+1}, e_k, \dots, e_1, e_0$ from ρ' to i in T (see Fig. 1), and we can infer the
 432 lengths of these edges in a ‘top-down’ approach (i.e., starting with edge e_{k+1} and moving
 433 down the tree towards edge e_0).

For $\ell(e_{k+1})$, let j be a leaf that is not a descendant of edge e_k (in other words, j is not in the same maximal pending subtree as i). Then, clearly,

$$PD_T(\{i, j\}) = PD_T(\{i\}) + PD_T(\{j\}) - \ell(e_{k+1}),$$

434 (because $\ell(e_{k+1})$ contributes twice to the sum $PD_T(\{i\}) + PD_T(\{j\})$, but only once to
 435 $PD_T(\{i, j\})$). In other words, $\ell(e_{k+1}) = PD_T(\{i\}) + PD_T(\{j\}) - PD_T(\{i, j\})$.

436 Now, let $e_i = (u, v)$ be an interior edge in the path from ρ' to i , for which the
 437 lengths of its preceding edges are already determined, i.e., $\ell(e_{k+1}), \dots, \ell(e_{i+1})$ are known.
 438 Moreover, let j be a leaf that is a descendant from e_i , but not from e_{i-1} .

Then, with a similar argument as in the previous case, we have

$$PD_T(\{i, j\}) = PD_T(\{i\}) + PD_T(\{j\}) - \ell(P(T; \rho', v)),$$

439 where $\ell(P(T; \rho', v))$ denotes the length of the unique path from ρ' to v in T (which
 440 contributes twice to the sum $PD_T(\{i\}) + PD_T(\{j\})$, but only once to $PD_T(\{i, j\})$). In

441 other words, $\ell(P(T; \rho', v)) = PD_T(\{i\}) + PD_T(\{j\}) - PD_T(\{i, j\})$. On the other hand,
442 $\ell(P(T; \rho', v)) = \ell(e_{k+1}) + \ell(e_k) + \dots + \ell(e_{i+1}) + \ell(e_i)$, and as $\ell(e_{k+1}), \dots, \ell(e_{i+1})$ are known,
443 we can uniquely infer $\ell(e_i)$.

444 Finally, after inferring the lengths of the edges e_{k+1}, e_k, \dots, e_1 as described above,
445 we can also uniquely infer the length of the pendant edge e_0 incident to i as

$$446 \ell(e_0) = PD_T(\{i\}) - \sum_{j=1}^{k+1} \ell(e_j).$$

447 In summary, we can uniquely infer all edge lengths of edges in the path from ρ' to i
448 from the PD scores of subsets of X of size at most 2. As i was an arbitrary leaf of T , this
449 completes the proof. □

450 *Proof of Theorem 2.*

451 Let \mathbb{F} be a feature assignment and let T be a rooted phylogenetic X -tree. First,
452 note that we can always achieve $\varphi_{\mathbb{F}}(x) = FP_{(T, \ell')}(x)$ for all $x \in X$ when we consider an
453 edge length assignment ℓ' that allows edges to be assigned length zero because, in this
454 case, if e_x denotes the pendant edge incident to x , we can set $\ell'(e_x) = \varphi_{\mathbb{F}}(x)$ for each
455 $x \in X$, and $\ell'(e) = 0$ for all interior edges and the stem edge, which clearly results in
456 $\varphi_{\mathbb{F}}(x) = FP_{(T, \ell')}(x)$ for all $x \in X$.

457 We now show that we can obtain an edge length assignment ℓ assigning strictly
458 positive lengths to all edges of T from ℓ' by redistributing lengths in a ‘bottom-up’
459 approach (i.e. moving from pendant edges towards the stem edge).

460 First, for each pendant edge e_x , set $\ell(e_x) = \ell'(e_x)$, which is strictly positive, due to
461 the assumed condition $F_x \neq \emptyset$, along with the fact that μ takes strictly positive values.
462 Now, let e be an edge of T such that all edges descending from e already have strictly
463 positive lengths, whereas all edges above e (if they exist) still have length zero. Let
464 e_1, \dots, e_k denote the descending edges incident to e , and let t_1, \dots, t_k denote the subtrees
465 pending from e (where tree t_i has stem edge e_i for $i = 1, \dots, k$). Moreover, for $i = 1, \dots, k$,
466 let $\delta_{e_i} := \frac{\ell(e_i)}{n(e_i)}$ denote the ratio between the length of e_i and the number of leaves
467 descending from it. Without loss of generality, we may assume that edge e_1 minimizes this

468 ratio (else we exchange edge labels). Furthermore, let $0 < c < 1$. We now re-assign edge
 469 lengths to e_1, \dots, e_k and e as follows (where $\ell_{\text{old}}(e_i)$ refers to the edge length e_i is currently
 470 assigned):

- 471 1. $\ell_{\text{new}}(e) := (1 - c) \cdot \ell_{\text{old}}(e_1) \cdot \frac{n(e)}{n(e_1)}$
- 472 2. $\ell_{\text{new}}(e_1) := c \cdot \ell_{\text{old}}(e_1)$,
- 473 3. $\ell_{\text{new}}(e_i) := \ell_{\text{old}}(e_i) - \frac{n(e_i)}{n(e)} \cdot \ell_{\text{new}}(e)$ for $i = 2, \dots, k$.

474 Now, in order to show that this is a valid re-distribution of edge lengths, we need to show
 475 that

- 476 (i) $\ell_{\text{new}}(e) > 0$ and $\ell_{\text{new}}(e_i) > 0$ for $i = 1, \dots, k$.
- 477 (ii) $FP_{(T, \ell_{\text{old}})}(x) = FP_{(T, \ell_{\text{new}})}(x)$ for all $x \in X$.

First, consider (i). As $\ell_{\text{old}}(e_1) > 0$ by assumption, and $0 < c < 1$, we clearly have
 $\ell_{\text{new}}(e) > 0$, and $\ell_{\text{new}}(e_1) > 0$. Now, consider e_i for $i \in \{2, \dots, k\}$. Here, we have

$$\begin{aligned}
 \ell_{\text{new}}(e_i) &= \ell_{\text{old}}(e_i) - \frac{n(e_i)}{n(e)} \cdot \ell_{\text{new}}(e) \\
 &= \ell_{\text{old}}(e_i) - \frac{n(e_i)}{n(e)} \cdot (1 - c) \cdot \ell_{\text{old}}(e_1) \cdot \frac{n(e)}{n(e_1)} \\
 &= \ell_{\text{old}}(e_i) - \frac{\ell_{\text{old}}(e_1)}{n(e_1)} \cdot n(e_i) \cdot (1 - c) \\
 &\geq \ell_{\text{old}}(e_i) - \frac{\ell_{\text{old}}(e_i)}{n(e_i)} \cdot n(e_i) \cdot (1 - c) \quad (\text{because } e_1 \text{ minimizes } \delta_{e_i} = \ell_{\text{old}}(e_i)/n(e_i)) \\
 &= \ell_{\text{old}}(e_i) - \ell_{\text{old}}(e_i) \cdot (1 - c) = c \cdot \ell_{\text{old}}(e_i) > 0,
 \end{aligned}$$

478 where the last inequality again follows from the fact that (by assumption) $\ell_{\text{old}}(e_i) > 0$ and
 479 $0 < c < 1$. This completes the proof of (i).

For (ii) note that the FP indices of taxa not descending from e are not affected by
 the re-assignment of edge lengths, so it suffices to consider all $x \in c_T(e)$. In the following,
 let $t_i \setminus e_i$ be the rooted phylogenetic tree obtained from t_i by deleting its stem edge. Then,

we clearly have for all $x \in c_T(e)$:

$$FP_{(T, \ell_{\text{old}})}(x) = FP_{(t \setminus e_i, \ell_{\text{old}})}(x) + \frac{\ell_{\text{old}}(e_i)}{n(e_i)},$$

(because by assumption all edges above e_i have length zero before the re-assignment of edge lengths according to steps 1–3). On the other hand, we have for all $x \in c_T(e)$:

$$FP_{(T, \ell_{\text{new}})}(x) = FP_{(t \setminus e_i, \ell_{\text{new}})}(x) + \frac{\ell_{\text{new}}(e_i)}{n(e_i)} + \frac{\ell_{\text{new}}(e)}{n(e)}.$$

Note that $FP_{(t \setminus e_i, \ell_{\text{old}})}(x) = FP_{(t \setminus e_i, \ell_{\text{new}})}(x)$ for all $x \in c_T(e)$ (because the lengths of edges in $t_i \setminus e_i$ are not changed). We now show that $FP_{(T, \ell_{\text{old}})}(x) = FP_{(T, \ell_{\text{new}})}(x)$ for all $x \in X$.

First, let $x \in t_1$. Then, we have

$$\begin{aligned} FP_{(T, \ell_{\text{new}})}(x) &= FP_{(t \setminus e_1, \ell_{\text{new}})}(x) + \frac{\ell_{\text{new}}(e_1)}{n(e_1)} + \frac{\ell_{\text{new}}(e)}{n(e)} \\ &= FP_{(t \setminus e_1, \ell_{\text{old}})}(x) + \frac{c \cdot \ell_{\text{old}}(e_1)}{n(e_1)} + \frac{(1-c) \cdot \ell_{\text{old}}(e_1) \cdot \frac{n(e)}{n(e_1)}}{n(e)} \\ &= FP_{(t \setminus e_1, \ell_{\text{old}})}(x) + c \cdot \frac{\ell_{\text{old}}(e_1)}{n(e_1)} + (1-c) \cdot \frac{\ell_{\text{old}}(e_1)}{n(e_1)} \\ &= FP_{(t \setminus e_1, \ell_{\text{old}})}(x) + \frac{\ell_{\text{old}}(e_1)}{n(e_1)} = FP_{(T, \ell_{\text{old}})}(x). \end{aligned}$$

Now, let $x \in t_i$ for $i \in \{2, \dots, k\}$. Then, we have

$$\begin{aligned} FP_{(T, \ell_{\text{new}})}(x) &= FP_{(t \setminus e_i, \ell_{\text{new}})}(x) + \frac{\ell_{\text{new}}(e_i)}{n(e_i)} + \frac{\ell_{\text{new}}(e)}{n(e)} \\ &= FP_{(t \setminus e_i, \ell_{\text{old}})}(x) + \frac{\ell_{\text{old}}(e_i) - \frac{n(e_i)}{n(e)} \cdot \ell_{\text{new}}(e)}{n(e_i)} + \frac{\ell_{\text{new}}(e)}{n(e)} \\ &= FP_{(t \setminus e_i, \ell_{\text{old}})}(x) + \frac{\ell_{\text{old}}(e_i)}{n(e_i)} - \frac{\ell_{\text{new}}(e)}{n(e)} + \frac{\ell_{\text{new}}(e)}{n(e)} \\ &= FP_{(T, \ell_{\text{old}})}(x). \end{aligned}$$

480 In summary, re-assigning edge lengths according to the conditions 1–3 (listed
 481 above) is valid (because conditions (i) and (ii) hold). Thus, for each edge e whose length
 482 was changed, we now simply set $\ell(e) = \ell_{\text{new}}(e)$ and repeat the procedure. In this way, we
 483 can construct an edge length assignment ℓ that assigns strictly positive lengths to *all* edges
 484 of T (including pendant edges and the stem edge), such that $\varphi_{\mathbb{F}}(x) = FP_{(T, \ell)}(x)$ for all
 485 $x \in X$. This completes the proof. □