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Phylogenetic beta diversity, similarity, and differentiation measures based on Hill numbers

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Abstract. Until now, decomposition of abundance-sensitive gamma (regional) phylogenetic diversity measures into alpha and beta (within- and between-group) components has been based on an additive partitioning of phylogenetic generalized entropies, especially Rao's quadratic entropy. This additive approach led to a phylogenetic measure of differentiation between assemblages: (gamma − alpha)/gamma. We show both empirically and theoretically that this approach inherits all of the problems recently identified in the additive partitioning of non-phylogenetic generalized entropies. When within-assemblage (alpha) quadratic entropy is high, the additive beta and the differentiation measure (gamma − alpha)/gamma always tend to zero (implying no differentiation) regardless of phylogenetic structures and differences in species abundances across assemblages. Likewise, the differentiation measure based on the phylogenetic generalization of Shannon entropy always approaches zero whenever gamma phylogenetic entropy is high. Such critical flaws, inherited from their non-phylogenetic parent measures (Gini-Simpson index and Shannon entropy respectively), have caused interpretational problems. These flaws arise because phylogenetic generalized entropies do not obey the replication principle, which ensures that the diversity measures are linear with respect to species addition or group pooling. Furthermore, their complete partitioning into independent components is not additive (except for phylogenetic entropy). Just as in the non-phylogenetic case, these interpretational problems are resolved by using phylogenetic Hill numbers that obey the replication principle. Here we show how to partition the phylogenetic gamma diversity based on Hill numbers into independent alpha and beta components, which turn out to be multiplicative. The resulting phylogenetic beta diversity (ratio of gamma to alpha) measures the effective number of completely phylogenetically distinct assemblages. This beta component measures pure differentiation among assemblages and thus can be used to construct several classes of similarity or differentiation measures normalized onto the range [0, 1]. We also propose a normalization to fix the traditional additive phylogenetic similarity and differentiation measures, and we show that this yields the same similarity and differentiation measures we derived from multiplicative phylogenetic diversity partitioning. We thus can achieve a consensus on phylogenetic similarity and differentiation measures, including *N*-assemblage phylogenetic generalizations of the classic Jaccard, Sørensen, Horn, and Morisita-Horn measures. Hypothetical and real examples are used for illustration.

Key words: beta diversity; differentiation; Hill numbers; phylogenetic diversity; phylogenetic entropy; quadratic entropy; replication principle; similarity.

Introduction

Measures of beta diversity, similarity, and differentiation are basic tools of ecological analyses (Magurran 2004, Magurran and McGill 2011). Most of these measures assume that all species are equally distinct, ignoring phylogenetic and functional differences between them. These measures hide the evolutionary dimension of assemblages. For example, these measures would show a maximal level of differentiation between the primate assemblages of Amazonia and Pacific South America, because these assemblages share no species. These measures would show the same high level of differentiation between the Amazonian and Madagascaran primate assemblages, since these also share no species. Yet, the first pair of assemblages share most genera and all subfamilies, and are derived from a relatively recent common ancestor, while the Amazonian/Madagascaran pair of assemblages share no genera or subfamilies, and have been on separate evolutionary paths for a much longer time. The phylogenetic depth of the differentiation between assemblages is obviously important for ecology, conservation biology, evolutionary theories of community assembly, and genetics. McPeek and Miller (1996), Webb (2000), Ricotta (2005*a*), Webb et al. (2006), Lozupone et al. (2007), Barcaro et

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al. (2007), Ferrier et al. (2007), Hardy and Senterre (2007), Bryant et al. (2008), Graham and Fine (2008), Faith et al. (2009), Pavoine et al. (2009), de Bello et al. (2010), Mouchet and Mouillot (2011), Weiher (2011) and Cavender-Bares et al. (2012), among others, have recognized the need for measures of phylogenetic differentiation that capture this depth of separation between groups to answer evolutionary and ecological questions, and to guide conservation policy. Such measures would be especially useful now that differences between species can be objectively quantified in the form of well-supported phylogenetic trees (Faith 1992, Warwick and Clarke 1995, Crozier 1997, Webb 2000, Ives and Helmus 2010, Pavoine et al. 2010, among others) or functional trees (Tilman 2001, Petchey and Gaston 2002, Weiher 2011, among others). Three special issues in *Ecology* featured a series of papers on integrating ecology and phylogenetics; see McPeek and Miller (1996), Webb et al. (2006), and Cavender-Bares et al. (2012), and papers in each issue.

Most previous phylogenetic similarity and differentiation measures were based on phylogenetic diversity indices such as Faith's widely used total branch length measure (Faith 1992), phylogenetic entropy (Allen et al. 2009), and Rao's quadratic entropy (Rao 1982), unified by Pavoine et al. (2009) into a family of phylogenetic generalized entropies. These are generalizations of their non-phylogenetic counterparts, species richness, Shannon entropy, Gini-Simpson index, and generalized entropies, respectively. Phylogenetic differentiation measures were obtained from these phylogenetic generalized entropies by additively partitioning them into within- and between-group (alpha and beta) components (Ricotta 2005*b*, Hardy and Senterre 2007, Pavoine et al. 2009, Mouchet and Mouillot 2011), following the traditional additive approach that had been applied to their non-phylogenetic counterparts (Lande 1996, Veech et al. 2002). The mean within-group or alpha value was subtracted from the regional or gamma value (the value for the pooled groups), and the resulting "beta" value, or its complement, was normalized by dividing by the gamma value. This was supposed to produce a normalized measure of differentiation or similarity.

Recently, however, researchers have discovered serious interpretational problems with this traditional additive partitioning approach when diversity is equated with Shannon entropy, the Gini-Simpson index, or most other generalized entropies (Jost 2006, 2007, Jost et al. 2010, Ellison 2010). The main measure of similarity in the additive approach, alpha/gamma, does not actually quantify the compositional similarity of the assemblages under study. This ratio can be arbitrarily close to unity (supposedly indicating high similarity) even when the assemblages being compared have no species in common. This problem arises because Shannon entropy, the Gini-Simpson index, and other generalized entropies do not satisfy the replication principle (Jost 2007), which we discuss in *Hill numbers obey the replication principle*. The phylogenetic generalizations of these measures, likewise, do not obey the replication principle, so they inherit this fundamental problem with the interpretation of the ratio alpha/gamma. The widely used Rao's quadratic entropy suffers from another problem: just like the Gini-Simpson index, Rao's quadratic entropy is nonadditive (it cannot be decomposed into the sum of independent within- and between-group components), so imposing an additive framework on it will produce a measure of "beta" that is confounded with within-group diversity (equivalently, with total diversity). As diversity increases, all these traditional abundance-sensitive differentiation measures approach fixed values independent of tree structure or differences in species abundances between assemblages, so they cease to be biologically informative. We prove all these points in *Fixing the additive "beta" of phylogenetic generalized entropies*, and illustrate them with examples.

The solution, just as in the non-phylogenetic case, is to convert the phylogenetic generalized entropies into phylogenetic Hill numbers, which do obey the replication principle. This has been done recently by Chao et al. (2010), Leinster and Cobbold (2012), and Scheiner (2012). We concentrate on Chao et al.'s mean phylogenetic diversity (described in the next section) because this measure can be directly applied to diversity decomposition. Many previous measures of phylogenetic diversity (e.g., Rao 1982, Faith 1992, Allen et al. 2009, Pavoine et al. 2009, Ricotta and Szeidl 2009, de Bello et al. 2010) turn out to be special cases or simple transformations of this mean phylogenetic diversity. Jost (2007) derived a partitioning method to decompose Hill numbers into independent components. Here, we modified his approach to a more general framework and derive a new alpha formula. We used this more general framework to obtain phylogenetic generalizations of alpha and beta diversity, and new phylogenetic generalizations of existing non-phylogenetic similarity and differentiation measures, such as the Jaccard, Sørensen, Horn, and Morisita-Horn similarity indices (Morisita 1959, Horn 1966) and C_{qN} overlap measures (Chao et al. 2008, 2012). We also show that some of the previous phylogenetic differentiation measures can be corrected by normalization to remove their dependency on the alpha value (or gamma value), and these normalized measures turn out to be identical to the phylogenetic generalizations of the overlap measures that we derive from partitioning phylogenetic Hill numbers. Thus, a consensus can be reached about measures of beta diversity, similarity, and differentiation that incorporates the information contained in a phylogenetic tree.

Phylogenetic Generalizations of Entropies and Hill Numbers

Generalized entropy

In order to understand the problems of previous phylogenetic diversity and differentiation measures, it is helpful to first understand the corresponding problems of non-phylogenetic generalized entropy measures. There are many families of generalized entropies. The generalized entropy most often used in ecology is the so-called Tsallis entropy:

$$ {}^{q}H = \left(1 - \sum_{i=1}^{S} p_i^q\right) \Big/ (q-1) \tag{1} $$

where $S \geq 1$ is the number of species in the assemblage, and p_i is the relative abundance of the ith species, with $i = 1, 2, \ldots, S$ (Havrda and Charvát 1967, Daróczy 1970, Tsallis 1988, Keylock 2005). When $q = 0$, ${}^{q}H$ becomes $S - 1$; when q tends to 1, ${}^{q}H$ tends to Shannon entropy ${}^{1}H = -\sum_{i=1}^{S} p_i \log p_i$. When $q = 2$, ${}^{q}H$ reduces to the Gini-Simpson index ${}^{2}H = 1 - \sum_{i=1}^{S} p_i^2$. The parameter q controls the sensitivity to species abundances. The measure with $q > 1$ is disproportionately sensitive to the abundant species, the measure with $0 \leq q < 1$ is disproportionately sensitive to the rare species, and the measure with $q = 1$ weighs all species by their frequency, without favoring either common or rare species. This interpretation of the order q is applicable to all families of measures discussed in this paper.

Jost (2006, 2007, 2010) and Jost et al. (2010) show that these measures have caused interpretational problems when equated with diversity. The changes in their magnitudes (for $q > 0$) are not linear with respect to species addition. Also, as mentioned in the *Introduction*, the ratio of alpha to gamma generalized entropies does not measure compositional similarity of the assemblages, and their partitioning is not additive (except when $q = 1$).

Phylogenetic generalized entropy

Pielou (1975) was the first to notice that the concept of diversity could be broadened to consider differences among species. The earliest taxonomic diversity measure is the *cladistic diversity* (CD), which is defined as the total number of nodes in a taxonomic tree that encompasses all of the species in the assemblage (Vane-Wright et al. 1991, Faith 1992). A more informative measure is Faith's phylogenetic diversity (PD; Faith 1992), which measures total branch length arising from the root node. In both CD and PD, species abundances are not considered.

Rao's *quadratic entropy* was the first diversity measure that accounted for both phylogeny and species abundances (Rao 1982):

$$ Q = \sum_{i,j} d_{ij} p_i p_j \tag{2a} $$

where d_{ij} denotes the phylogenetic distance (in years since divergence, number of DNA base changes, or other metrics) between species i and j. It is an extension of the Gini-Simpson index, and reduces to it in the special case of no phylogenetic structure (all species are equally related to one another), $d_{ii} = 0$ and $d_{ij} = 1$ $(i \neq j)$. The *phylogenetic entropy* H_p extends Shannon entropy to incorporate phylogenetic distances among species (Allen et al. 2009) as follows:

$$ H_P = -\sum_i L_i a_i \log a_i \tag{2b} $$

where the summation is over all branches of a rooted phylogenetic tree, L_i is the length of branch i, and a_i denotes the summed relative abundance of all species descended from branch i.

For ultrametric trees, Pavoine et al. (2009) showed that Faith's PD, Allen et al.'s (2009) H_p, and Rao's Q can be united into a single parametric family of *phylogenetic generalized entropies*:

$$ {}^{q}I(T) = \left(T - \sum_{i \in \mathbf{B}_T} L_i a_i^q\right) \Big/ (q-1). \tag{2c} $$

Here, $\mathbf{B}_T$ is the set of all branches in the time interval $[-T, 0]$, and L_i and a_i are defined in Eq. 2b. Pavoine et al. (2009) only considered T equal to the age of the root of the phylogenetic tree. For notational consistency with Hill numbers and for comparison with our phylogenetic measure described in *Phylogenetic Hill numbers*, which allow arbitrary values of T, we use the notation ${}^{q}I(T)$ instead of the original notation I_q used in Pavoine et al. (2009).

This phylogenetic generalized entropy has a simple interpretation in terms of ordinary non-phylogenetic generalized entropies ${}^{q}H$ (Eq. 1). We can slice an ultrametric phylogenetic tree at any time t (for details, see Chao et al. 2010: Fig. 1), and from this perspective at time t, we can look at how the individuals in the assemblage are grouped into taxa. From the perspective of time t, the number of distinct taxa in the present assemblage is the number of branch cuts at time t, and the relative importance of each of these virtual taxa in the present-day assemblage is the sum of the relative abundances of the branch's descendants in the present-day assemblage. The ordinary non-phylogenetic generalized entropy ${}^{q}H$ can be calculated for each slice, using these relative importance values as the relative abundances p_i. These ordinary generalized entropies can be integrated over time, from the base of the tree (time $= -T$, not necessarily the root) to its tips (the present time). Since the generalized entropies are constant in any interval of time that contains no nodes, it will be easy to integrate if we divide the tree into M intervals, with each node defining an interval boundary, so that intervals have no internal nodes. The interval boundaries, which are the node ages, are labeled $\{t_0, \ldots, t_k, \ldots, t_M\}$, starting at the most basal interval (so that $t_0 = -T$, and

$t_M = 0$); see Appendix A for an example. Then, the integral simplifies to a simple sum of the ordinary generalized entropies (${}^qH_k$, $k = 1, 2, \ldots, M$) in the M intervals, weighted by the duration of that interval. This sum is

$$ {}^qI(T) = \sum_{k=1}^{M} (t_k - t_{k-1})({}^qH_k) \tag{2d}$$

which is equivalent to Eq. 2c. In order to be consistent with our own measures and the graphs in our examples, we reversed the ordering of the intervals used by Pavoine et al. (2009), who indexed the intervals from tips to root. If T is chosen as the age of the root node of the tree, then ${}^0I(T)$ = Faith's PD minus the tree height; ${}^1I(T)$ is identical to Allen et al.'s (2009) entropy H_p; and ${}^2I(T)$ is identical to Rao's quadratic entropy Q. In the special case of $M = 1$ (all lineages are completely distinct, i.e., there are no internal nodes) and $T = 1$, the phylogenetic generalized entropy reduces to the classical generalized entropy defined in Eq. 1 with species relative abundances $\{p_1, p_2, \ldots, p_S\}$ as the tip node relative abundances.

Hill numbers obey the replication principle

Hill (1973) proposed a class of diversity measures called "Hill numbers," or "effective number of species," defined for $q \neq 1$ as

$$ {}^qD = \left(\sum_{i=1}^{S} p_i^q \right)^{1/(1-q)}. \tag{3}$$

The parameter q determines the sensitivity of the measure to the species abundances. When $q = 0$, the abundances of individual species do not contribute; only presences are counted, so that ${}^0D$ is simply species richness. Eq. 3 is undefined for $q = 1$, but its limit as q tends to 1 is the exponential of Shannon entropy, i.e., ${}^1D = \exp({}^1H)$. ${}^1D$ weighs species in proportion to their frequency. When $q = 2$, ${}^2D$ is the inverse Simpson concentration and places more weight on the frequencies of abundant species and discounts rare species. Investigators should at least report the diversity for all species ($q = 0$), the typical species ($q = 1$), and the dominant species ($q = 2$).

All Hill numbers are in units of "species." It is thus possible to plot them on a single graph as a continuous function of the parameter q. A complete characterization of the species diversity of an assemblage with S species and relative abundances ($p_1, p_2, \ldots, p_S$) is conveyed by a diversity profile: a plot of ${}^qD$ vs. q from $q = 0$ to $q = 4$ or 5 (beyond this it changes little); see Tóthmérész (1995). An example of a diversity profile is shown in Appendix B. Although Hill numbers for $q < 0$ can be calculated, they are dominated by the frequencies of rare species and have poor statistical sampling properties. We thus restrict ourselves to the case $q \geq 0$ throughout the paper.

Hill numbers differ fundamentally from generalized entropies in that they are linear with respect to species addition or group pooling. That is, they obey the replication principle: When N completely distinct assemblages with identical diversities of order q are pooled in equal proportions, the diversity of the pooled assemblage is N times the diversity of any single assemblage. The N completely distinct assemblages may have different relative abundances (and, for $q > 0$, they can even have different numbers of species). See Appendix B for proof. This property is the strong replication principle (a weaker one was proven by Hill 1973). Because Hill numbers obey this replication principle, changes in their magnitude have simple interpretations, and the ratio of alpha diversity to gamma diversity accurately reflects the similarity of the assemblages.

Phylogenetic Hill numbers

Since generalized entropies do not obey the replication principle, neither do their phylogenetic generalizations. This can be solved by transforming them into Hill numbers, which obey the replication principle. Chao et al. (2010) generalized Hill numbers to take phylogenies into account for all values of q. Define $\mathbf{B}_T$, L_i, and a_i as in Eqs. 2b and 2c. Chao et al. (2010) derived the *mean phylogenetic diversity for the interval* $[-T, 0]$ (or mean diversity over T years) as

$$ {}^q\bar{D}(T) = \left\{ \sum_{i \in \mathbf{B}_T} \frac{L_i}{T} a_i^q \right\}^{1/(1-q)} = \frac{1}{T} \left\{ \sum_{i \in \mathbf{B}_T} L_i \left(\frac{a_i}{T} \right)^q \right\}^{1/(1-q)} \qquad q \geq 0 \text{ and } q \neq 1 \tag{4a}$$

$$ {}^1\bar{D}(T) = \lim_{q \to 1} {}^q\bar{D}(T) = \exp\left[-\sum_{i \in \mathbf{B}_T} \frac{L_i}{T} a_i \log a_i \right]. \tag{4b}$$

It is interpreted as the effective number of completely distinct lineages (no shared lineages) during the time interval from T years ago to the present.

This mean diversity is invariant to the units used to measure branch lengths. There is a simple relationship between our measures and Rao's quadratic entropy Q, ${}^2\bar{D}(T) = 1/(1 - Q/T)$, and likewise between our measure and Allen et al.'s (2009) phylogenetic entropy H_p, ${}^1\bar{D}(T) = \exp(H_p/T)$. See Chao et al. (2010) for a proof. When lineages are completely distinct over the time interval $[-T, 0]$ (so that all branch lengths are equal to T, and thus, all lineages are equally distinct), the mean diversity ${}^q\bar{D}(T)$ reduces to the non-phylogenetic Hill numbers ${}^qD = (\sum_i a_i^q)^{1/(1-q)}$. This includes the special case when T tends to zero, which means that we ignore phylogeny and only consider the present-day assemblage.

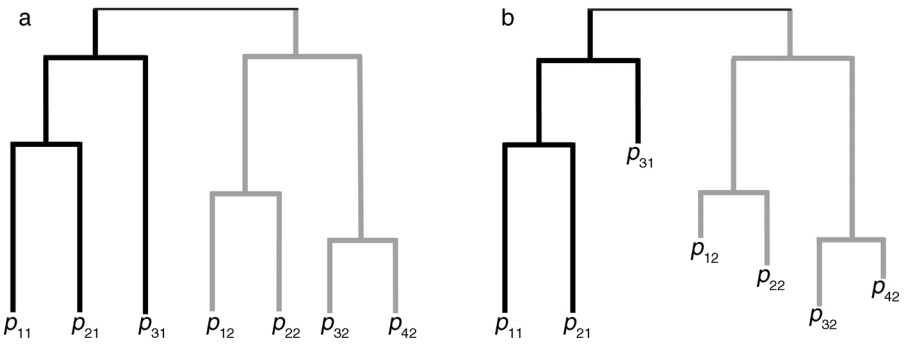

FIG. 1. Replication principle for two completely phylogenetically distinct assemblages with totally different structures. (a) Assemblage 1 (black) includes three species with species relative abundances $\{p_{11}, p_{21}, p_{31}\}$ for the three tips. Assemblage 2 (gray) includes four species with species relative abundances $\{p_{12}, p_{22}, p_{32}, p_{42}\}$ for the four tips. The diversity of the pooled tree is double of that of each tree as long as the two assemblages are completely phylogenetically distinct as shown (no lineages shared between assemblages, though lineages within an assemblage may be shared) and have identical mean diversities. (b) The same is valid for two completely phylogenetically distinct non-ultrametric assemblages.

The *branch or phylogenetic diversity* ${}^{q}\mathrm{PD}(T)$ of order q during the time interval from T years ago to the present is defined as the product of ${}^{q}\bar{D}(T)$ and T. That is, ${}^{q}\mathrm{PD}(T) = T \times {}^{q}\bar{D}(T)$, which quantifies the amount of evolutionary "work" done on the system over the interval $[-T, 0]$, or the effective number of lineage-years (or other tree units) contained in the tree on the interval $[-T, 0]$. If $q = 0$, ${}^{0}\mathrm{PD}(T)$ reduces to Faith's phylogenetic diversity, regardless of abundances. Two types of profiles completely characterize phylogenetic diversity. (1) A diversity profile is obtained by plotting ${}^{q}\mathrm{PD}(T)$ or ${}^{q}\bar{D}(T)$ as functions of T for $q = 0$, 1, and 2; see Fig. B2 (Appendix B) or Chao et al. (2010: Fig. 3) for examples. (2) The other type of diversity profile is obtained by plotting ${}^{q}\mathrm{PD}(T)$ or ${}^{q}\bar{D}(T)$ as a function of order q, for a selected value of temporal perspective T. See Fig. B3 (Appendix B) for examples.

In many applications, the measure of evolutionary work is based on the number of nucleotide base changes at a selected locus, or the amount of functional or morphological differentiation from a common ancestor. In these cases, the lengths from tips to the root of the phylogenetic tree are not necessarily all equally long, so the tree is not ultrametric. In these cases, the time parameter T should be replaced by $\bar{T}$, the weighted arithmetic mean of the distances from the tree base to each of the terminal branch tips (i.e., the mean evolutionary change per species over the interval of interest):

$$\bar{T} = \sum_{i \in \mathbf{B}_{\bar{T}}} L_i a_i.$$

In other words, $\bar{T}$ is the mean tree height. Here, $\mathbf{B}_{\bar{T}}$ denotes the set of branches connecting the chosen tree base to all the branch tips (species) in the assemblage. See Fig. 1 in Chao et al. (2010) for an illustrative example. As shown by Chao et al. (2010), the mean phylogenetic diversity and branch diversity for a non-ultrametric assemblage have the same form as those for an ultrametric tree, except that T must be replaced by the mean tree height $\bar{T}$ (if abundance data are available so that it can be obtained). Therefore, if the diversity of a non-ultrametric assemblage is z, then its diversity is the same as the diversity of an ultrametric assemblage consisting of z equally abundant and completely distinct lineages all with branch length $\bar{T}$. Although our derivation and presentation for the rest of the paper are focused on ultrametric trees, all results and conclusions for our proposed measures are also valid for non-ultrametric trees if $\bar{T}$ is substituted for T.

Unlike previous phylogenetic diversity measures developed in the literature, the mean diversity and the amount of evolutionary work done on the assemblage depend explicitly on T, the temporal perspective of the investigator. However, the time T does not need to be the age of the oldest node; it may be less (though this would throw away phylogenetic information and would rarely be done) or it may be greater than the age of the root node. Often, the most appropriate and least arbitrary choice is the divergence time between the group under study and its nearest outgroup; the sampling protocol (for example, the decision to keep orchids but not other families) uniquely determines this number. This contrasts with the traditional approach using the root node as the reference point. In that approach, the age of the root node can depend on the vagaries of sampling success, so the traditional phylogenetic measures will often change with sampling effort, and cannot be directly compared between studies. Diversities of different assemblages should generally be compared using the same T for all of them. It is easy to convert results to different T values; see the *Discussion*.

Phylogenetic Hill numbers obey the replication principle

The replication principle for Hill numbers can be generalized to phylogenetic diversity in the following sense: when we combine N equally weighted, completely phylogenetically distinct assemblages (no lineages

shared among assemblages in the interval $[-T, 0]$; see Fig. 1), each with the same mean diversity ${}^{q}\bar{D}(T) = X$ in the time interval $[-T, 0]$, the pooled assemblages must have mean diversity ${}^{q}\bar{D}(T) = N \times X$. Also, the amount of evolutionary work ${}^{q}\mathrm{PD}(T)$ done on the pooled assemblages is N times the amount of evolutionary work done on a single assemblage. The same temporal perspective T (or for non-ultrametric trees, the same mean quantity $\bar{T}$) must be used for all N assemblages, but they may have different numbers of species and totally different tree structures. Most previous phylogenetic diversity measures do not obey the replication principle, but the phylogenetic Hill numbers proposed here do obey it. See Appendix B or Chao et al. (2010) for proofs. This intuitive property sets our phylogenetic diversity measures apart from the phylogenetic generalized entropy measures.

Partitioning Hill Numbers and their Phylogenetic Generalizations into Alpha and Beta Components

Partitioning Hill numbers into alpha and beta components

The formulas for alpha, beta, and gamma depend on the question under investigation. We consider a fixed set of N assemblages. The total diversity of the pooled assemblage (gamma diversity) can be decomposed multiplicatively into independent alpha and beta components. Assume that there are S species in the pooled assemblages. Let $y_{ij} \geq 0$ denote any measure of species importance of the ith species in the jth assemblage, $i = 1, 2, \ldots, S$, $j = 1, 2, \ldots, N$. Throughout the paper, we will refer to y_{ij} as measures of "abundance." They can be absolute abundances, relative abundances, incidence, or any other importance measure (e.g., biomass, coverage of plants or corals, basal area of plants). Any transformation of these measures can also be used for y_{ij}; see Lengendre and Legendre (2012) for various transformations. Our goal was to quantify the species-by-species resemblance or differentiation of the N sets of abundances, $(y_{1j}, y_{2j}, \ldots, y_{Sj})$, $j = 1, 2, \ldots, N$.

Let $y_{++} = \sum_{i=1}^{S}\sum_{j=1}^{N} y_{ij}$ be the total abundance in the region, and let $y_{+j} = \sum_{i=1}^{S} y_{ij}$ be the assemblage size of the jth assemblage. In order to link our approach to previous work in the literature, we first re-express the value y_{ij} as

$$y_{ij} = y_{++}\left(\frac{y_{+j}}{y_{++}}\right)\left(\frac{y_{ij}}{y_{+j}}\right) \equiv y_{++} w_j p_{ij} \tag{5a}$$

where $p_{ij} = y_{ij}/y_{+j}$ is the relative abundance of the ith species in the jth assemblage, and $w_j = y_{+j}/y_{++}$ (relative assemblage size or the *weight* of the jth assemblage), with $\sum_{j=1}^{N} w_j = 1$. Thus, comparing the N sets of vectors $(y_{1j}, y_{2j}, \ldots, y_{Sj})$, $j = 1, 2, \ldots, N$, is equivalent to comparing the N sets of vectors $(w_j p_{1j}, w_j p_{2j}, \ldots, w_j p_{Sj})$, $j = 1, 2, \ldots, N$. If our goal is to compare the N sets of relative abundance vectors $(p_{1j}, p_{2j}, \ldots, p_{Sj})$, $j = 1, 2, \ldots, N$, we can simply define y_{ij} to be the species relative abundance in the jth assemblage. In this special case, $y_{+j} = 1$, $y_{++} = N$, then assemblage weight naturally becomes $1/N$, an equal-weight case.

For the gamma diversity, we simply pool species abundances over assemblages, and let $y_{i+} = \sum_{j=1}^{N} y_{ij} = y_{++}\sum_{j=1}^{N} w_j p_{ij}$ be the total value of the ith species in the region. The gamma diversity of order q is the Hill number based on the relative abundance $\bar{p}_{i+} = y_{i+}/y_{++} = \sum_{j=1}^{N} w_j p_{ij}$ in the pooled assemblage (Routledge 1979, Jost 2006, 2007) as follows:

$${}^{q}D_{\gamma} = \left\{\sum_{i=1}^{S}\left(\frac{y_{i+}}{y_{++}}\right)^{q}\right\}^{1/(1-q)} = \left\{\sum_{i=1}^{S}\left(\sum_{j=1}^{N} w_j p_{ij}\right)^{q}\right\}^{1/(1-q)} \qquad q \neq 1. \tag{5b}$$

When q tends to 1, we have

$${}^{1}D_{\gamma} = \lim_{q\to 1} {}^{q}D_{\gamma} = \exp\left\{-\sum_{i=1}^{S}(y_{i+}/y_{++})\log(y_{i+}/y_{++})\right\} = \exp\left\{-\sum_{i=1}^{S}\left(\sum_{j=1}^{N} w_j p_{ij}\right)\log\left(\sum_{j=1}^{N} w_j p_{ij}\right)\right\}. \tag{5c}$$

In Appendix C, we derive the following new formula for alpha diversity, which is interpreted as "the effective number of species per assemblage":

$${}^{q}D_{\alpha} = \frac{1}{N}\left\{\sum_{i=1}^{S}\sum_{j=1}^{N}\left(\frac{y_{ij}}{y_{++}}\right)^{q}\right\}^{1/(1-q)} = \frac{1}{N}\left\{\sum_{i=1}^{S}\sum_{j=1}^{N}(w_j p_{ij})^{q}\right\}^{1/(1-q)} \qquad q \neq 1. \tag{6a}$$

The formula when q tends to 1 is

$${}^{1}D_{\alpha} = \lim_{q\to 1} {}^{q}D_{\alpha} = \exp\left\{-\sum_{i=1}^{S}\sum_{j=1}^{N}(y_{ij}/y_{++})\log(y_{ij}/y_{++}) - \log N\right\} = \exp\left\{-\sum_{i=1}^{S}\sum_{j=1}^{N} w_j p_{ij}\log(w_j p_{ij}) - \log N\right\}. \tag{6b}$$

For any arbitrary weights, our gamma is always greater than or equal to the alpha for *all* orders $q \geq 0$. The beta component is ${}^{q}D_{\beta} = {}^{q}D_{\gamma}/{}^{q}D_{\alpha}$, which is always between unity (when all assemblages are identical in species absolute abundances) and N (when the N assemblages have no species in common); see Appendix C for proofs. The beta diversity can be interpreted as the effective number of completely distinct assemblages in the region (i.e., assemblage diversity).

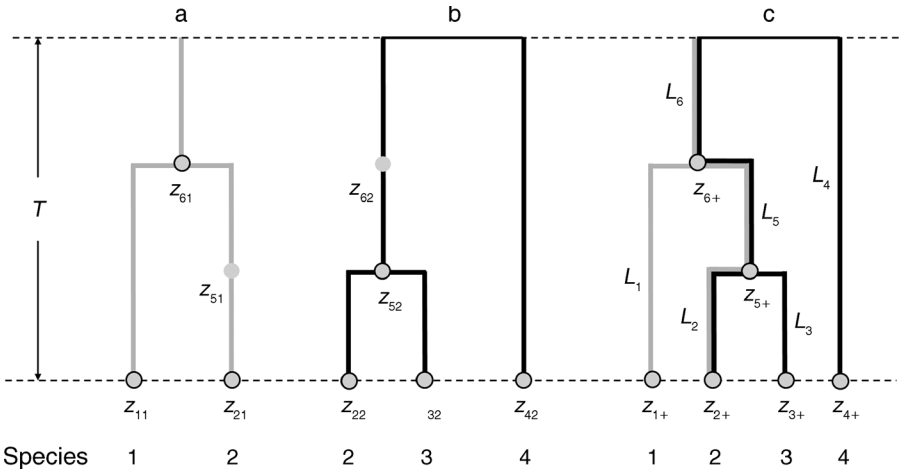

FIG. 2. (a) Phylogenetic tree for assemblage 1 (gray) with species (1, 2) and tip node abundance (z_{11}, z_{21}). (b) Phylogenetic tree for assemblage 2 (black) with species (2, 3, 4) and tip node abundance (z_{22}, z_{32}, z_{42}). The variable z_{ij} can be species absolute abundance, species relative abundance in the jth assemblage, any other quantitative variables, or any transformation of the above measures. (c) Pooled tree for four species (1, 2, 3, 4) with four tip node abundance (z_{1+}, z_{2+}, z_{3+}, z_{4+}) and the corresponding branch lengths (L_1, L_2, L_3, L_4), and two internal-node abundance (z_{5+}, z_{6+}) with branch lengths (L_5, L_6). Suppose the weights (the relative sizes of assemblages) for assemblages 1 and 2 are w_1 and w_2, respectively. The whole pooled phylogenetic tree in the time interval $[-T, 0]$ includes six nodes and their corresponding branch lengths. Based on the branch set and branch lengths in the pooled tree, the diversity of the pooled assemblage is calculated by using the node abundance set $(z_{1+}, z_{2+}, z_{3+}, z_{4+}, z_{5+}, z_{6+}) = (z_{11}, z_{21} + z_{22}, z_{32}, z_{42}, z_{21} + z_{22} + z_{32}, z_{11} + z_{21} + z_{22} + z_{32})$ with the corresponding branch lengths (L_1, L_2, L_3, L_4, L_5, L_6). The diversity of assemblage 1 can be calculated by using the pooled tree with the node abundance set (z_{11}, z_{21}, 0, 0, z_{21}, $z_{11} + z_{21}$). The diversity of assemblage 2 can be calculated by using the pooled tree with tip node abundance set (0, z_{22}, z_{32}, z_{42}, $z_{22} + z_{32}$, $z_{22} + z_{32}$). The similarity between the two assemblages measures the node-by-node resemblance between the two node abundance sets (z_{11}, z_{21}, 0, 0, z_{21}, $z_{11} + z_{21}$) and (0, z_{22}, z_{32}, z_{42}, $z_{22} + z_{32}$, $z_{22} + z_{32}$). The non-phylogenetic similarity measures the species-by-species resemblance between the two tip node abundance sets (z_{11}, z_{21}, 0, 0) and (0, z_{22}, z_{32}, z_{42}). Gray closed dots represent nodes in each tree. When the phylogenetic tree of each individual assemblage is embedded in the pooled tree, one additional node (gray open circle) is added so that the diversity of each individual assemblage can be simply computed from the pooled tree structure.

Routledge (1979) and Jost (2007) each derived a mathematical formula for alpha diversity. For equal-weight case, all the three alpha formulas are identical. They differ, however, when assemblage weights are not equal due to different assumptions used in deriving each alpha formula. These three alpha formulas will be compared elsewhere. Previous approaches to alpha diversity led to a beta that can only be used to produce differentiation measures to compare species *relative* abundances, but not absolute abundances. Our approach expands the conventional concept of alpha so that beta can quantify the differentiation among N sets of vectors $(y_{1j}, y_{2j}, \ldots, y_{Sj})$ $j = 1, 2, \ldots, N$ for any measure of species importance y_{ij}, including absolute abundances. See Appendix C for the mathematical properties of our proposed new alpha and beta diversities.

Our alpha component is independent of beta and contains only the within-group information, and the beta component contains only the between-group information. Neither component, taken by itself, imposes any mathematical constraints on the other component; if we know only the value of one component, we cannot infer anything about the other component. This ensures that beta is not confounded with alpha, an essential prerequisite for much biological reasoning about diversity and differentiation. The precise meaning of independence for alpha and beta components has been the subject of debate and misunderstanding (e.g., Baselga 2010, Ellison 2010, Jost 2010, Ricotta 2010, Veech and Crist 2010); see Chao et al. (2012) for a detailed resolution.

Partitioning mean phylogenetic diversity into alpha and beta components

The mean phylogenetic diversity ${}^{q}\bar{D}(T)$ (Eqs. 4a and 4b) can be decomposed into independent phylogenetic alpha and beta diversities. Here, we take into account the phylogenetic distances among species in comparing assemblages. We need to introduce some additional notation conventions for phylogenetic trees. See Fig. 2 for an example. A pooled tree is first constructed for the regional assemblage. For this pooled assemblage in the time interval $[-T, 0]$, define $\mathbf{B}_T$ as the set of all branches, and L_i be the length of branch i, $i \in \mathbf{B}_T$. The tip nodes represent those species in the present-day assemblage. For the jth assemblage, $j = 1, 2, \ldots, N$, let z_{ij} denote the total abundances descended from branch i, $i \in \mathbf{B}_T$, although z_{ij} can be any quantitative measure of species importance as discussed in the preceding section. (Here, the index i can correspond to both tip node and internal node; if i is a tip node, then z_{ij} represents data of the current assemblage and is analogous to y_{ij} in *Partitioning Hill*

numbers into alpha and beta components). As shown in Fig. 2, the diversity for each individual assemblage can be easily computed from the pooled tree structure. Only the node abundances vary with assemblages.

Our goal here is to quantify the node-by-node resemblance (or differentiation) among the N abundance sets $\{z_{ij};\, i \in \mathbf{B}_T\}$, $j = 1, 2, \ldots, N$. Let $a_{ij} = z_{ij}/z_{+j}$ (here the "+" sign in z_{+j} denotes a sum over the tip nodes only) be the corresponding relative abundances descended from branch i in the jth assemblage, and $z_{++} = \sum_{j=1}^{N} z_{+j}$. For the pooled assemblage, it follows from Eq. 5a that we have a similar expression, $z_{ij} = z_{++} w_j a_{ij}$ where $w_j = z_{+j}/z_{++}$ (relative assemblage size) is the weight for the jth assemblage. In the pooled assemblage, the node abundance for branch i becomes $z_{i+} = z_{++} \sum_{j=1}^{N} w_j a_{ij}$, and the corresponding relative abundance is $\bar{a}_{i+} = z_{i+}/z_{++} = \sum_{j=1}^{N} w_j a_{ij}$.

The phylogenetic gamma diversity of order q can be calculated from Eq. 4a as

$$
\begin{aligned}
{}^{q}\bar{D}_{\gamma}(T) &= \frac{1}{T}\left\{\sum_{i\in\mathbf{B}_T} L_i \left(\frac{z_{i+}/z_{++}}{T}\right)^{q}\right\}^{1/(1-q)} \\
&= \frac{1}{T}\left\{\sum_{i\in\mathbf{B}_T} L_i \left(\frac{\sum_{j=1}^{N} w_j a_{ij}}{T}\right)^{q}\right\}^{1/(1-q)} \\
& \qquad q \geq 0 \text{ and } q \neq 1. \qquad (7a)
\end{aligned}
$$

The limit when q approaches unity exists and is equal to

$${}^{1}\bar{D}_{\gamma}(T) = \lim_{q\to 1} {}^{q}\bar{D}_{\gamma}(T) = \exp\left[-\sum_{i\in\mathbf{B}_T} \frac{L_i}{T}\left(\sum_{j=1}^{N} w_j a_{ij}\right)\log\left(\sum_{j=1}^{N} w_j a_{ij}\right)\right]. \qquad (7b)$$

The gamma diversity is the effective number of completely distinct lineages over the interval $[-T, 0]$ in the pooled assemblage. In Appendix C, we derive the following phylogenetic alpha diversity for $q \geq 0$ and $q \neq 1$ as

$$
\begin{aligned}
{}^{q}\bar{D}_{\alpha}(T) &= \frac{1}{TN}\left\{\sum_{i\in\mathbf{B}_T} L_i \sum_{j=1}^{N}\left(\frac{z_{ij}/z_{++}}{T}\right)^{q}\right\}^{1/(1-q)} \\
&= \frac{1}{TN}\left\{\sum_{i\in\mathbf{B}_T} L_i \sum_{j=1}^{N}\left(\frac{w_j a_{ij}}{T}\right)^{q}\right\}^{1/(1-q)}. \qquad (8a)
\end{aligned}
$$

For $q = 1$, we have

$$
\begin{aligned}
{}^{1}\bar{D}_{\alpha}(T) &= \lim_{q\to 1} {}^{q}\bar{D}_{\alpha}(T) \\
&= \exp\left[-\sum_{i\in\mathbf{B}_T} L_i \sum_{j=1}^{N} \frac{w_j a_{ij}}{T}\log\frac{w_j a_{ij}}{T} - \log(NT)\right]. \qquad (8b)
\end{aligned}
$$

The alpha diversity is interpreted as the effective number of completely distinct lineages over the interval $[-T, 0]$ for an individual assemblage.

Gamma diversity should not be smaller than alpha diversity. As in the case of our non-phylogenetic decomposition of Hill numbers, our phylogenetic gamma (Eqs. 7a and 7b) and alpha (Eqs. 8a and 8b) components satisfy this property for *all* $q \geq 0$ and any arbitrary weights (see Appendix C). The complete partitioning of phylogenetic gamma diversity into independent within- and between-group (alpha and beta) diversities is multiplicative. The phylogenetic beta diversity is the ratio of gamma diversity to alpha diversity:

$${}^{q}\bar{D}_{\beta}(T) = \frac{{}^{q}\bar{D}_{\gamma}(T)}{{}^{q}\bar{D}_{\alpha}(T)} \qquad q \geq 0. \qquad (9)$$

This is equivalent to the ratio of gamma branch diversity to alpha branch diversity, i.e., ${}^{q}\bar{D}_{\beta}(T) = {}^{q}\mathrm{PD}_{\gamma}(T)/{}^{q}\mathrm{PD}_{\alpha}(T)$. When the N assemblages are identical in species identities and species abundances, then ${}^{q}\bar{D}_{\beta}(T) = 1$ for any T. When the N assemblages are completely phylogenetically distinct (no shared lineages), then ${}^{q}\bar{D}_{\beta}(T) = N$, no matter what the diversities or tree shapes of the assemblages. The phylogenetic beta diversity ${}^{q}\bar{D}_{\beta}(T)$ quantifies assemblage diversity and is the effective number of completely phylogenetically distinct assemblages in the interval $[-T, 0]$. See Fig. 1 for examples of completely phylogenetically distinct assemblages. This interpretation is conceptually the same as the beta diversity for ordinary Hill numbers, but incorporates the relatedness of species. When all lineages in the pooled assemblage are completely distinct in the interval $[-T, 0]$, the phylogenetic alpha, beta, and gamma diversities reduce to those based on ordinary Hill numbers. This includes the limiting case that T tends to zero, so that phylogeny is ignored. If our goal is to quantify the node-by-node resemblance among the N relative abundance sets $\{a_{ij};\, i \in \mathbf{B}_T\}$, $j = 1, 2, \ldots, N$, then we just redefine z_{ij} to be a_{ij}, implying that assemblage weights become equal ($w_j = 1/N$) in Eqs. 7a, 7b, 8a, 8b, and 9.

When $q = 0$, we have ${}^{0}\bar{D}_{\beta}(T) = L_{\gamma}(T)/L_{\alpha}(T)$, where $L_{\gamma}(T)$ denotes the total branch length of the pooled tree, and $L_{\alpha}(T)$ denotes the average length of an individual tree. When $q = 1$, the phylogenetic beta diversity of order 1 is

$${}^{1}\bar{D}_{\beta}(T) = \exp[(H_{P,\gamma} - H_{P,\alpha})/T + \sum_{j=1}^{N} w_j \log w_j + \log N] \qquad (10a)$$

where $H_{P,\gamma}$ and $H_{P,\alpha}$ denote, respectively, the gamma and alpha phylogenetic entropy. When assemblage weights are equal, this implies an additive decomposition for phylogenetic entropy H_P (Pavoine et al. 2009, Mouchet and Mouillot 2011), as for ordinary Shannon entropy (Jost 2007). When $q = 2$ and

assemblages are equally weighted, the phylogenetic beta diversity of order 2 is as follows (see Appendix C for proof):

$$^{2}\bar{D}_{\beta}(T) = (1 - Q_{\gamma}/T)^{-1}/(1 - Q_{\alpha}/T)^{-1} \qquad (10b)$$

where Q_{γ} and Q_{α} denote, respectively, the gamma and alpha quadratic entropy.

Since our alpha and gamma phylogenetic diversities both obey the replication principle, the beta diversity formed by taking their ratio is replication-invariant (see Appendix C for proof). That is, when assemblages are replicated, the beta diversity does not change. This property is related to the condition that alpha and beta must be independent. A consequence is that beta can be easily converted into normalized similarity and differentiation measures by transformations that do not depend on alpha or gamma diversity. We make use of this property in the following section. Another consequence is consistency when pooling equally distinct sub-trees, such as pooling equally ancient subfamilies. If all subfamilies show the same beta diversity, the beta diversity is unchanged by pooling the subfamilies.

As with ordinary Hill numbers, the *lineage excess* $^{q}\bar{D}_{\gamma}(T) - {}^{q}\bar{D}_{\alpha}(T)$ can be interpreted as the effective number of regional lineages not contained in a typical local assemblage, or the absolute number of lineages gained in going from the local to the regional scale. The lineage excess and the phylogenetic beta together contain the same information as phylogenetic alpha and gamma diversities. The measure $[^{q}\bar{D}_{\gamma}(T) - {}^{q}\bar{D}_{\alpha}(T)]/(N - 1)$ quantifies the lineage turnover rate per assemblage (i.e., the effective number of lineages unique to a typical local assemblage). The relative lineage turnover rate per assemblage can be measured by $[^{q}\bar{D}_{\gamma}(T) - {}^{q}\bar{D}_{\alpha}(T)]/[(N - 1)(^{q}\bar{D}_{\alpha}(T))] = [^{q}\bar{D}_{\beta}(T) - 1]/(N - 1)$ This is one class of measures proposed in the next section.

Normalized Similarity/Differentiation Measures and Their Phylogenetic Generalizations

Normalized similarity/differentiation measures based on Hill numbers

Based on the gamma diversity (Eqs. 5b and 5c) and the new alpha formula (Eqs. 6a and 6b), our beta diversity as a ratio of gamma and alpha is independent of alpha and always lies in the range $[1, N]$ for any arbitrary weights and all orders $q \geq 0$ (Appendix C). Since the range depends on N, the beta diversity cannot be used to compare species differentiation across multiple regions with different numbers of assemblages. To remove the dependence on N, we follow Jost (2006, 2007) and Chao et al. (2008, 2012), who proposed several transformations to measure local overlap, regional overlap, homogeneity, and turnover. A summary of these non-phylogenetic measures and their relationship with previous measures is shown in Table 1. See Appendix D for details.

This framework reveals that many of the most popular measures in an ecologist's toolbox, including the Jaccard, Sørensen, Horn, and Morisita-Horn measures of similarity for two assemblages (Morisita 1959, Horn 1966), are transformations of multiplicative beta diversity. The multiplicative beta diversity can be calculated for any number of assemblages, so the beta-transformation viewpoint led to multiple-assemblage generalizations of the classic measures (Jost 2006, 2007, Chao et al. 2008). Nearly all of the previous similarity measures in the literature based on Hill numbers can only be used for comparing relative abundances. For all $q \geq 0$, our new beta diversity using the new alpha formula (Eq. 6a) is valid for any weights, so the beta-transformation viewpoint also leads to one kind of weighted generalizations of the classic measures. This enables us to compare absolute abundance sets (by using relative sizes as assemblage weights), in addition to relative abundance sets (by using equal weights). As Clarke and Warwick (2001) concluded, a suitable similarity (or differentiation) measure should have the flexibility to reflect resemblance (or difference) in absolute abundances, not just relative abundances; see also Magurran (2004:174). Anderson et al. (2006:692) also indicated "... differences in absolute abundances can also be important ecologically, as they may correspond to differences in an ecosystem's productivity or responses to a pollutant or other impact."

Phylogenetic generalizations of normalized similarity/differentiation measures

Since our phylogenetic beta diversity has the same mathematical properties as the multiplicative beta diversity based on ordinary Hill numbers, we can now generalize all of those non-phylogenetic similarity measures in Table 1 to include phylogenetic similarities between assemblages. All of the transformation formulas are still valid, with the ordinary multiplicative beta diversity replaced by our phylogenetic beta diversity (which is a function of T, the temporal perspective of the investigator). Of course, all these measures are also mathematically independent of alpha diversity, a property that most existing phylogenetic similarity measures lack.

Table 2 summarizes the four classes of phylogenetic similarity measures derived from our approach. The corresponding differentiation measures are the one-complements of the similarity measures. The formulas for the special cases for $q = 0$, 1, and 2 are also displayed there. All derivation details are provided in Appendix D, and a brief description is given below:

1. *Lineage overlap from a local perspective*.—This class of measures takes the following form:

$$\bar{C}_{qN}(T) = \frac{N^{1-q} - [^{q}\bar{D}_{\beta}(T)]^{1-q}}{N^{1-q} - 1}. \qquad (11a)$$

TABLE 1. Four classes of non-phylogenetic similarity measures and their special cases, based on the beta diversity from partitioning Hill numbers.

Measure	Turnover-complement $V_{qN} = \dfrac{N - {}^{q}D_{\beta}}{N-1}$	Homogeneity measure $S_{qN} = \dfrac{1/{}^{q}D_{\beta} - 1/N}{1-1/N}$
$q = 0$	Sørensen $\dfrac{N - S/\bar{S}}{N-1}$	Jaccard $\dfrac{\bar{S}/S - 1/N}{1-1/N}$
$q = 1$ (equal weight)	...	...
$q = 1$ (general weight)	...	...
$q = 2$ (equal weight)	Regional-overlap $1 - \dfrac{H_{GS,\gamma} - H_{GS,\alpha}}{(N-1)(1-H_{GS,\gamma})}$	Morisita-Horn $1 - \dfrac{H_{GS,\gamma} - H_{GS,\alpha}}{(1-1/N)(1-H_{GS,\alpha})}$
$q = 2$ (general weight)	$1 - \dfrac{\sum_{i=1}^{S}\sum_{j>k}^{N}(w_j p_{ij} - w_k p_{ik})^2}{(N-1)\sum_{i=1}^{S}\bar{p}_{i+}^2}$	$1 - \dfrac{\sum_{i=1}^{S}\sum_{j>k}^{N}(w_j p_{ij} - w_k p_{ik})^2}{(N-1)\sum_{i=1}^{S}\sum_{j=1}^{N}w_j^2 p_{ij}^2}$

Notes: The corresponding differentiation measures are the one-complements of the similarity measures. To quantify the resemblance of absolute abundance sets, use relative assemblage sizes as weights; to quantify the resemblance of relative abundance sets, use equal weight. ${}^{q}D_{\beta} = {}^{q}D_{\gamma}/{}^{q}D_{\alpha}$, where ${}^{q}D_{\gamma} = \{\sum_{i=1}^{S}(\sum_{j=1}^{N} w_j p_{ij})^q\}^{1/(1-q)}$, ${}^{q}D_{\alpha} = (1/N)\{\sum_{i=1}^{S}\sum_{j=1}^{N}(w_j p_{ij})^q\}^{1/(1-q)}$; p_{ij} is the relative abundance of the ith species in the jth assemblage; w_j is the relative assemblage size; and $\bar{p}_{i+} = \sum_{j=1}^{N} w_j p_{ij}$; see Eqs. 5b, 5c, 6a, and 6b for details (in subsection *Partitioning Hill numbers into alpha and beta components*). $\bar{S}$ is the alpha species richness (average species richness per assemblage); H_{γ} and H_{α} are gamma and alpha Shannon entropy, respectively; and $H_{GS,\gamma}$ and $H_{GS,\alpha}$ are gamma and alpha Gini-Simpson indices, respectively. Ellipses (...) indicate that the equation is not displayed because it cannot be linked to any other conventional measures.

TABLE 2. Four classes of phylogenetic similarity measures and their special cases, based on the phylogenetic beta diversity from partitioning mean phylogenetic diversity.

Measure	Phylo-turnover-complement, $\tilde{V}_{qN}(T) = \dfrac{N - {}^{q}\tilde{D}_{\beta}(T)}{N-1}$	Phylo-homogeneity, $\tilde{S}_{qN}(T) = \dfrac{1/{}^{q}\tilde{D}_{\beta}(T) - 1/N}{1-1/N}$
$q = 0$	Phylo- Sørensen $\dfrac{N - L_{\gamma}(T)/L_{\alpha}(T)}{N-1}$	Phylo-Jaccard $\dfrac{L_{\alpha}(T)/L_{\gamma}(T) - 1/N}{1-1/N}$
$q = 1$ (equal weight)	...	...
$q = 1$ (general weight)	...	...
$q = 2$ (equal weight)	Phylo-regional-overlap $1 - \dfrac{Q_{\gamma} - Q_{\alpha}}{(N-1)(T - Q_{\gamma})}$	Phylo-Morisita-Horn $1 - \dfrac{Q_{\gamma} - Q_{\alpha}}{(1-1/N)(T - Q_{\alpha})}$
$q = 2$ (general weight)	$1 - \dfrac{\sum_{i\in\mathbf{B}_T} L_i \sum_{j>k}^{N}(w_j a_{ij} - w_k a_{ik})^2}{(N-1)\sum_{i\in\mathbf{B}_T} L_i \bar{a}_{i+}^2}$	$1 - \dfrac{\sum_{i\in\mathbf{B}_T} L_i \sum_{j>k}^{N}(w_j a_{ij} - w_k a_{ik})^2}{(N-1)\sum_{i\in\mathbf{B}_T} L_i \sum_{j=1}^{N} w_j^2 a_{ij}^2}$

Notes: The corresponding differentiation measures are the one-complements of the similarity measures. When all lineages are completely distinct (this includes $T \to 0$, ignoring phylogeny), the phylogenetic measures reduces to the corresponding non-phylogenetic versions in Table 1. (All measures can also be applied to non-ultrametric trees if $\bar{T}$ is substituted for T.) First row: All measures are functions of ${}^{q}\bar{D}_{\beta}(T)$, where ${}^{q}\bar{D}_{\beta}(T) = {}^{q}\bar{D}_{\gamma}(T)/{}^{q}\bar{D}_{\alpha}(T)$, ${}^{q}\bar{D}_{\gamma}(T) = (1/T)\{\sum_{i\in\mathbf{B}_T} L_i(\sum_{j=1}^{N} w_j a_{ij}/T)^q\}^{1/(1-q)}$, and ${}^{q}\bar{D}_{\alpha}(T) = [1/(TN)]\{\sum_{i\in\mathbf{B}_T} L_i \sum_{j=1}^{N}(w_j a_{ij}/T)^q\}^{1/(1-q)}$. Here, $\mathbf{B}_T$ is the set of all branches in the time interval $[-T, 0]$; L_i is the length of branch i; a_{ij} is the the total relative abundance descended from branch i in the jth assemblage; w_j is relative assemblage size for quantifying the resemblance of species absolute abundances among assemblages ($w_j = 1/N$ for quantifying the resemblance of species relative abundances); and $\bar{a}_{i+} = \sum_{j=1}^{N} w_j a_{ij}$; see Eqs. 7a, 7b, 8a, and 8b for details (in the subsection *Partitioning mean phylogenetic diversity into alpha and beta components*). Second row: $L_{\gamma}(T)$ and $L_{\alpha}(T)$ are, respectively, the gamma and alpha Faith's phylogenetic diversity (PD; total lineage length). Third and fourth rows: $H_{p,\gamma}$ and $H_{p,\alpha}$ are the gamma and alpha phylogenetic entropy. Fifth row: Q_{γ} and Q_{α} are the gamma and alpha quadratic entropy. Ellipses (...) indicate that the equation is not displayed because it cannot be linked to any other conventional measures.

TABLE 1. Extended.

Local-overlap $C_{qN} = \dfrac{(1/{}^{q}D_{\beta})^{q-1} - (1/N)^{q-1}}{1-(1/N)^{q-1}}$	Regional-overlap $U_{qN} = \dfrac{(1/{}^{q}D_{\beta})^{1-q} - (1/N)^{1-q}}{1-(1/N)^{1-q}}$
Sørensen $\dfrac{N - S/\bar{S}}{N-1}$	Jaccard $\dfrac{\bar{S}/S - 1/N}{1-1/N}$
Horn overlap $1 - \dfrac{H_{\gamma} - H_{\alpha}}{\log N}$	Horn overlap $1 - \dfrac{H_{\gamma} - H_{\alpha}}{\log N}$
$\dfrac{H_{\alpha} - H_{\gamma} - \sum_{j=1}^{N} w_j \log w_j}{\log N}$	$\dfrac{H_{\alpha} - H_{\gamma} - \sum_{j=1}^{N} w_j \log w_j}{\log N}$
Morisita-Horn $1 - \dfrac{H_{GS,\gamma} - H_{GS,\alpha}}{(1-1/N)(1-H_{GS,\alpha})}$	Regional-overlap $1 - \dfrac{H_{GS,\gamma} - H_{GS,\alpha}}{(N-1)(1-H_{GS,\gamma})}$
$1 - \dfrac{\sum_{i=1}^{S}\sum_{j>k}^{N}(w_j p_{ij} - w_k p_{ik})^2}{(N-1)\sum_{i=1}^{S}\sum_{j=1}^{N} w_j^2 p_{ij}^2}$	$1 - \dfrac{\sum_{i=1}^{S}\sum_{j>k}^{N}(w_j p_{ij} - w_k p_{ik})^2}{(N-1)\sum_{i=1}^{S} \bar{p}_{i+}^2}$

It gives the effective average proportion of shared lineages in an individual assemblage. This class of similarity measures extends the C_{qN} overlap measure derived in Chao et al. (2008) to phylogenetic and weighted versions. If N assemblages each have S equally common and completely distinct lineages in the interval $[-T, 0]$, with exactly A lineages shared by all of them, and the remaining lineages of each assemblage are not shared by any other assemblages, then $\bar{C}_{qN}(T)$ gives the lineage overlap A/S for all orders of q. The differenti-

TABLE 2. Extended.

Phylo-local-overlap $\tilde{C}_{qN}(T) = \dfrac{[1/{}^{q}\bar{D}_{\beta}(T)]^{q-1} - (1/N)^{q-1}}{1-(1/N)^{q-1}}$	Phylo-regional-overlap $\tilde{U}_{qN}(T) = \dfrac{[1/{}^{q}\bar{D}_{\beta}(T)]^{1-q} - (1/N)^{1-q}}{1-(1/N)^{1-q}}$
Phylo-Sørensen $\dfrac{N - L_{\gamma}(T)/L_{\alpha}(T)}{N-1}$	Phylo-Jaccard $\dfrac{L_{\alpha}(T)/L_{\gamma}(T) - 1/N}{1-1/N}$
Phylo-Horn overlap $1 - \dfrac{H_{p,\gamma} - H_{p,\alpha}}{T\log N}$	Phylo-Horn overlap $1 - \dfrac{H_{p,\gamma} - H_{p,\alpha}}{T\log N}$
$\dfrac{H_{P,\alpha} - H_{P,\gamma} - T\sum_{j=1}^{N} w_j \log w_j}{T\log N}$	$\dfrac{H_{P,\alpha} - H_{P,\gamma} - T\sum_{j=1}^{N} w_j \log w_j}{T\log N}$
Phylo-Morisita-Horn $1 - \dfrac{Q_{\gamma} - Q_{\alpha}}{(1-1/N)(T-Q_{\alpha})}$	Phylo-regional-overlap $1 - \dfrac{Q_{\gamma} - Q_{\alpha}}{(N-1)(T-Q_{\gamma})}$
$1 - \dfrac{\sum_{i\in\mathbf{B}_T} L_i \sum_{j>k}^{N}(w_j a_{ij} - w_k a_{ik})^2}{(N-1)\sum_{i\in\mathbf{B}_T} L_i \sum_{j=1}^{N} w_j^2 a_{ij}^2}$	$1 - \dfrac{\sum_{i\in\mathbf{B}_T} L_i \sum_{j>k}^{N}(w_j a_{ij} - w_k a_{ik})^2}{(N-1)\sum_{i\in\mathbf{B}_T} L_i \bar{a}_{i+}^2}$

ation measure $1 - \bar{C}_{qN}(T)$ thus quantifies the effective average proportion of unique lineages in an assemblage.

For $q = 0$, this similarity measure is referred to as the "phylo-Sørensen" N-assemblage overlap measure because for $N = 2$, it reduces to the measure *PhyloSor* (phylo-Sørensen) developed by Bryant et al. (2008) and Ferrier et al. (2007). For $q = 1$, this measure $\bar{C}_{1N}(T)$ is called the "phylo-Horn" N-assemblage overlap measure because it extends Horn (1966) two-assemblage measure to incorporate phylogenies and weights for N assemblages. For $q = 2$, $\bar{C}_{2N}(T)$ is called the "phylo-Morisita-Horn" N-assemblage similarity measure because it extends Morisita-Horn measure (Morisita 1959) to incorporate phylogenies and weights for N assemblages. The differentiation measure $1 - \bar{C}_{2N}(T)$ for the equal-weight case reduces to the measure proposed by de Bello et al. (2010). Their measure is valid only for ultrametric trees (de Bello et al. 2010: 7). For $q = 2$, Eq. 11a as applied to equally weighted non-ultrametric trees reduces to the following (see Table 2):

$$1 - \bar{C}_{2N}(\bar{T}) = \frac{1 - [1/{}^{2}\bar{D}_{\beta}(\bar{T})]}{1 - 1/N} = \frac{Q_{\gamma} - Q_{\alpha}}{(1 - 1/N)(\bar{T} - Q_{\alpha})} \tag{11b}$$

where Q_{γ} and Q_{α} are, respectively, gamma and alpha quadratic entropy, and $\bar{T}$ is the mean base change. This is the phylogenetic generalization of Jost's (2008) genetic differentiation measure D. See the *Discussion* for more informtion about its application to genetics. A general form taking into account assemblage weights (so that absolute abundances can be compared) is

$$1 - \bar{C}_{2N}(\bar{T}) = \frac{\sum_{i \in \mathbf{B}_{\bar{T}}} L_i \sum_{j>k}^{N} (w_j a_{ij} - w_k a_{ik})^2}{(N-1) \sum_{i \in \mathbf{B}_{\bar{T}}} L_i \sum_{j=1}^{N} w_j^2 a_{ij}^2}. \tag{11c}$$

This generalizes Jost's measure D to assess differences in both phylogenies and assemblage weights. The above expression shows that the similarity index $\bar{C}_{2N}(\bar{T})$, as in all our similarity measures, is unity if and only if $w_j a_{ij} = w_k a_{ik}$ (i.e., absolute abundances are identical) for all node i in the branch set and for any two assemblages j and k. This reveals that the index compares *absolute* abundances node by node among the N assemblages. Therefore, when absolute abundances differ, there can be nonzero differentiation even if all assemblages have identical species *relative* abundances. If our target is to compare node-by-node relative abundances, we simply change our measure of species importance to relative abundances and thus equal weights are naturally obtained. Then the differentiation index is zero if and only if all assemblages have identical node-by-node relative abundances.

2. *Lineage overlap from a regional perspective*.—This class of measures takes the form

$$\bar{U}_{qN}(T) = \frac{[1/{}^{q}\bar{D}_{\beta}(T)]^{1-q} - (1/N)^{1-q}}{1 - (1/N)^{1-q}}. \tag{12a}$$

This class of measures quantifies the effective proportion of shared lineages in the pooled assemblage. Assume each of the N assemblages has only completely distinct lineages and the phylogenetic trees for all assemblages are identical. If there are S completely distinct, equally abundant lineages in the pooled assemblage, with exactly R lineages shared by all N assemblages, and with the remaining $S - R$ lineages evenly distributed in N assemblages, then this measure equals the lineage overlap R/S in the pooled assemblage. In this case, the measure $1 - \bar{U}_{qN}(T) = 1 - R/S$ is a complementarity measure for all orders of q.

For $q = 0$, this measure is called the "phylo-Jaccard" N-assemblage measure because for $N = 2$ the measure $1 - \bar{U}_{02}(T)$ reduces to the Jaccard-type *UniFrac* measure developed by Lozupone and Knight (2005) and the PD-dissimilarity measure developed by Faith et al. (2009). For $q = 1$, this measure is identical to the "phylo-Horn" N-assemblage overlap measure $\bar{C}_{1N}(T)$; see Table 2. For $q = 2$, we refer to the measure $\bar{U}_{2N}(T)$ as a "phylo-regional-overlap" measure. For equally weighted non-ultrametric trees, we have

$$1 - \bar{U}_{2N}(\bar{T}) = \frac{N - {}^{2}\bar{D}_{\beta}(\bar{T})}{N - 1} = \frac{Q_{\gamma} - Q_{\alpha}}{(N-1)(\bar{T} - Q_{\gamma})}.$$

See Table 2 for a more general formula with assemblage weights.

3. *Phylogenetic homogeneity*.—This class of measures takes the form

$$\bar{S}_{qN}(T) = \frac{1/{}^{q}\bar{D}_{\beta}(T) - 1/N}{1 - 1/N} \tag{12b}$$

This measure is linear in the proportion of regional diversity contained in the typical assemblage. For $q = 0$, it is the "phylo-Jaccard" N-assemblage measure $\bar{U}_{0N}(T)$. For $q = 2$, this measure is identical to $\bar{C}_{2N}(T)$, the "phylo-Morisita-Horn" N-assemblage similarity measure. Thus, we have $\bar{S}_{0N}(T) = \bar{U}_{0N}(T)$ and $\bar{S}_{2N}(T) = \bar{C}_{2N}(T)$ see Table 2. However, for $q = 1$, this measure does not reduce to the "phylo-Horn" overlap measure.

4. *Complement of phylogenetic turnover rate*.—This class of measures takes the form

$$\bar{V}_{qN}(T) = \frac{N - {}^{q}\bar{D}_{\beta}(T)}{N - 1} = 1 - \frac{{}^{q}\bar{D}_{\beta}(T) - 1}{N - 1}. \tag{12c}$$

The corresponding differentiation measure $[{}^{q}\bar{D}_{\beta}(T) - 1]/(N - 1)$ is the relative lineage turnover rate per assemblage. This differentiation measure is linear in beta and measures the relative lineage turnover rate per assemblage. When $q = 0$, the measure $\bar{V}_{0N}(T)$ is identical to the "phylo-Sørensen" N-assemblage measure. For $q = 2$, this measure is identical to $\bar{U}_{2N}(T)$, the "phylo-regional-overlap" measure. That is, we have $\bar{V}_{0N}(T) = \bar{C}_{0N}(T)$ and $\bar{V}_{2N}(T)$

$= \bar{U}_{2N}(T)$; see Table 2. However, for $q = 1$, this measure does not reduce to the "phylo-Horn" overlap measure.

All these measures are continuous as q ranges from zero to infinity, so a similarity or dissimilarity profile can be made for any of them. We suggest using this method for conveying complete information about the similarity of a set of assemblages (Jost et al. 2011). An example will be given in *Example 3: A real phylogenetic tree for rockfish*.

Although the lineage excess ${}^{q}\bar{D}_{\gamma}(T) - {}^{q}\bar{D}_{\alpha}(T)$ is a useful measure, it cannot be directly applied to compare the similarity or differentiation across multiple regions because it depends on the number of assemblages, and also on the mean phylogenetic alpha (equivalently, gamma) diversity. Following Chao et al. (2012), we can easily eliminate these dependences by using an appropriate normalization. In Appendix D, we show that after proper normalizations, the phylogenetic beta diversity and the lineage excess both lead to the same four classes of normalized similarity and differentiation measures as those in Table 2.

Fixing the additive "beta" of phylogenetic generalized entropies

The traditional approach to partitioning quadratic entropy Q (in Eq. 2a), phylogenetic entropy H_p (in Eq. 2b), and phylogenetic generalized entropy ${}^{q}I(T)$ (in Eq. 2c) has been additive. Here, we demonstrate the mathematical flaws of the additive approach based on ${}^{q}I(T)$, for $q = 2$ (quadratic entropy) and $q = 1$ (phylogenetic entropy). Since the "beta" quadratic entropy is related to our measure only in the equal-weight case (Table 2), we focus on the equal-weight case and show how to fix them and connect the additive approach to our measures.

In the traditional approach, the additive "beta" is defined as the phylogenetic generalized entropy excess (gamma minus alpha entropies), ${}^{q}I_{\beta}(T) = {}^{q}I_{\gamma}(T) - {}^{q}I_{\alpha}(T)$. This excess is usually converted into a normalized "differentiation" measure as

$$J_{qN}(T) = {}^{q}I_{\beta}(T)/{}^{q}I_{\gamma}(T) = 1 - {}^{q}I_{\alpha}(T)/{}^{q}I_{\gamma}(T) \qquad (13a)$$

or a "similarity" measure is constructed as $1 - J_{qN}(T) = {}^{q}I_{\alpha}(T)/{}^{q}I_{\gamma}(T)$. (Here, we put the order q as a subscript for the two measures $J_{qN}(T)$ and $1 - J_{qN}(T)$ in order to compare it with our phylogenetic similarity measures $\bar{C}_{qN}(T)$ and $\bar{U}_{qN}(T)$).

However, gamma generalized entropy cannot be additively partitioned into independent within- and between-group components for $q \neq 1$ (Jost 2007), and this nonadditivity also applies to phylogenetic generalized entropies. Additive "beta" phylogenetic generalized entropy is constrained by alpha phylogenetic generalized entropy through the inequality

$$0 \leq {}^{q}I_{\beta}(T) \leq \frac{(1 - N^{1-q})\{T - (q-1)[{}^{q}I_{\alpha}(T)]\}}{q-1}, \qquad q \neq 1. \qquad (13b)$$

For $q = 1$, the corresponding inequality is

$$0 \leq {}^{1}I_{\beta}(T) \leq \lim_{q \to 1} \frac{(1 - N^{1-q})\{T - (q-1)[{}^{q}I_{\alpha}(T)]\}}{q-1} = T \log N. \qquad (13c)$$

See Appendix E for proofs. When all species are completely distinct and $T = 1$, the measure ${}^{q}I(T)$ reduces to the generalized entropy (in Eq. 1), so Eq. 13b reduces to its non-phylogenetic version (Jost et al. 2010). These inequalities show why the traditional phylogenetic similarity and differentiation measures produce counterintuitive results, and also how to fix them. We discuss the three most commonly used special cases ($q = 0, 1, 2$).

1. $q = 2$.—Eq. 13b shows that the "beta" quadratic entropy Q_{β} is confounded with alpha quadratic entropy Q_{α} through the constraint $Q_{\beta} \leq (1 - 1/N)(T - Q_{\alpha})$. A high alpha quadratic entropy means that $Q_{\alpha} \to T$, so that additive "beta" is necessarily to be small, even if the assemblages share no lineages whatsoever. This implies that, when Q_{α} is high (close to T), the "differentiation" measure $J_{2N}(T)$ is necessarily going close to 0, and the "similarity" measure $1 - J_{2N}(T)$ is close to its maximum value of unity, for *any* set of assemblages, even assemblages that share no species or lineages. So the additive "beta" does not measure pure differentiation among assemblages, and the "similarity" and "differentiation" measures also do not really measure phylogenetic similarity and differentiation. The low values do not reflect reality, but are inescapable mathematical consequences of Eq. 13b. In *Examples* we demonstrate this by means of hypothetical and real examples, and compare the measure $J_{2N}(T)$ with our proposed measures. See Hardy and Senterre (2007) for another real example; in this case, the authors later recognized the problem and rectified their interpretation (Hardy and Jost 2008). To fix this problem, the upper bound in Eq. 13b can be used to construct a normalized measure in the range [0, 1]. As shown in Table 2 and Eq. 11b, the normalized measure $Q_{\beta}/[(1 - 1/N)(T - Q_{\alpha})]$ is exactly our differentiation measure $1 - \bar{C}_{2N}(T)$.

2. $q = 1$.—It follows from the inequality Eq. 13c that additive "beta" phylogenetic entropy is bounded by $T \log N$, if N and T are both fixed. Thus, additive "beta" is not constrained by alpha, and additive "beta" and alpha are independent (not confounded), as in the non-phylogenetic case. This can be also seen from Eq. 10a for the equal-weight case. However, since additive "beta" is bounded by $T \log N$, it follows that the differentiation measure $J_{1N}(T)$ ("beta"/gamma) is always close to 0 if the denominator gamma tends to be large, regardless of the true differentiation. In this case, the similarity measure $1 - J_{1N}(T)$ (i.e., alpha/gamma) is always close to unity. Thus, even though for $q = 1$, additive decomposition based on phylogenetic entropy is justified (as in the non-phylogenetic Shannon entropy), the normalized measure $J_{1N}(T)$ still cannot quantify differentiation, and its complement still does not reflect similarity. This happens because Shannon entropy does

not obey the replication principle. The upper bound in Eq. 13c reveals that phylogenetic entropy additive "beta" should be normalized not by gamma, but by $T \log N$ instead. This is clearly seen from Table 2 (for $q = 1$), and when this "beta" is normalized by this constant, our differentiation measure $1 - \bar{C}_{1N}(T)$ is obtained.

3. $q = 0$.—It follows from the inequality Eq. 13b that additive "beta" based on Faith's total branch length $L(T)$ is bounded by $(N-1)[T + {}^0I_\alpha(T)] = (N-1)L_\alpha(T)$, so that the additive "beta" is positively constrained by alpha. The normalized differentiation measure using (lineage excess)/gamma is $[L_\gamma(T) - L_\alpha(T)]/L_\gamma(T) = (1 - 1/N)(1 - \bar{U}_{0N}(T))$, where $\bar{U}_{0N}(T)$ is the "phylo-Jaccard" similarity measure (Table 2). The resulting measure is a legitimate differentiation measure, but it ranges from 0 (when all assemblages are identical) to $1-1/N$ (when all assemblages have no shared lineages). We propose dividing the additive "beta" by its maximum value to obtain a normalized measure $[L_\gamma(T) - L_\alpha(T)]/[(N-1)L_\alpha(T)]$, which is identical to our differentiation measure $1 - \bar{C}_{0N}(T)$ with range [0, 1].

As shown in Eq. 13b, the traditional "beta" phylogenetic generalized entropy for $q > 1$ is *negatively* constrained by the value of alpha, and for $q < 1$ it is *positively* constrained by the value of alpha. Thus, the anomalous behavior is also present for all other values of q. These anomalous behaviors can be easily fixed by using proper normalizations. For all orders $q \neq 1$, the dependence of the phylogenetic "beta" on its alpha can be removed by dividing the additive "beta" ${}^qI_\beta(T)$ by its maximum possible value in Eq. 13b. In Appendix E, we prove for all T that this "beta" ${}^qI_\beta(T)$, when properly normalized so as to remove its dependence on alpha, yields the same normalized differentiation measure $1 - \bar{C}_{qN}(T)$ (and normalized similarity measure $\bar{C}_{qN}(T)$) as the multiplicative partitioning scheme applied to mean phylogenetic diversity.

The dependence relationship in Eq. 13b is equivalent to the following constraint which shows how the additive "beta" phylogenetic generalized entropy ${}^qI_\beta(T)$ depends on gamma phylogenetic generalized entropy

$$0 \leq {}^qI_\beta(T) \leq \frac{(1/N^{1-q} - 1)\{T - (q-1)[{}^qI_\gamma(T)]\}}{q-1} \quad q \neq 1. \tag{13d}$$

For $q = 1$, a similar upper bound $T \log N$ is also obtained as in Eq. 13c. Similar conclusions and implications as those for Eq. 13b can be obtained. We omit the details. For all orders $q \neq 1$, if we normalize the "beta" phylogenetic generalized entropy ${}^qI_\beta(T)$ by its maximum in Eq. 13d, then the normalized measure yields the normalized differentiation measure $1 - \bar{U}_{qN}(T)$, a "true complementarity" measure from a regional view. The extension of Eqs. 13b, 13c, and 13d to the general non-ultrametric cases is provided in Appendix E.

The three measures (phylogenetic beta diversity, lineage excess, and phylogenetic generalized entropies) all lead to the two classes of normalized phylogenetic similarity measures $\bar{C}_{qN}(T)$ (a true local lineage overlap) and $\bar{U}_{qN}(T)$ (a true regional lineage overlap), as well as their corresponding differentiation measures. Thus, we finally achieve a consensus on the issue of normalized phylogenetic similarity and differentiation measures; see Table 2. We suggest using two types of profiles to characterize the proposed differentiation measures $1 - \bar{C}_{qN}(T)$ and $1 - \bar{U}_{qN}(T)$. (1) For a fixed order q (including at least 0, 1, and 2), the first type of profile is obtained by plotting our differentiation measures as a function of time perspective T. (2) For any fixed time perspective T (including at least $T = 0$ and $T =$ the age of the root of the pooled tree), the second type of profile is obtained by plotting our differentiation measures with respect to the order q. See *Examples* for illustrative plots and *Discussion* for the choices of T and q.

Examples

In all examples, we consider three phylogenetic measures: $J_{qN}(T) = 1 - {}^qI_\alpha(T)/{}^qI_\gamma(T)$ (based on phylogenetic generalized entropy, Eq.13a), $1 - \bar{C}_{qN}(T)$, and $1 - \bar{U}_{qN}(T)$ (both are based on our mean phylogenetic diversity) to quantify the differentiation between two assemblages. For comparisons, we also consider the non-phylogenetic versions of these measures: J^*_{qN} (based on generalized entropy), $1 - C_{qN}$ and $1 - U_{qN}$ (based on Hill numbers); see Table 1 for all measures.

Example 1: A simple hypothetical tree with completely distinct lineages

To decide whether our proposed similarity and differentiation measures are more appropriate than the "similarity" and "differentiation" measures based on traditional additive partitioning of quadratic entropy and phylogenetic entropy, we will first apply all measures to very simple trees for which unequivocal answers exist. If a phylogenetic similarity or differentiation measures cannot yield logical and sensible results for simple trees, we would not expect it to work for complicated real trees.

Consider two assemblages of landlocked organisms that originated on a super-continent that broke into two parts. For simplicity, suppose all species in each assemblage began to diverge from their common ancestor very soon after separation of the continents T years ago, and suppose each species is equally common so that the two assemblages are equally weighted. (Nothing important hinges on this latter assumption, which simplifies calculation.) The assemblages evolved in isolation for approximately T years. See Appendix F for an illustrative figure and derivation details.

For this example ($N = 2$), our proposed normalized phylogenetic differentiation measures $1 - \bar{C}_{qN}(T)$ and $1 - \bar{U}_{qN}(T)$ are always 1 for any q, any richnesses S, and any values of T; see Table 3. This value of unity correctly indicates that we have two maximally distinct

TABLE 3. Non-phylogenetic and phylogenetic differentiation measures between two assemblages for three examples, where T = age of the root node.

	Differentiation measures between two assemblages					
	Non-phylogenetic			Phylogenetic		
Order q	$1 - C_{qN}$	$1 - U_{qN}$	J^*_{qN}	$1 - \bar{C}_{qN}(T)$	$1 - \bar{U}_{qN}(T)$	$J_{qN}(T)$
Example 1						
$q = 0$	1	1	0.53	1	1	0.53
$q = 1$	1	1	0.23	1	1	0.23
$q = 2$	1	1	0.05	1	1	0.05
Example 2						
$q = 0$	0.76	0.86	0.44	0.66	0.79	0.41
$q = 1$	0.76	0.76	0.15	0.63	0.63	0.16
$q = 2$	0.76	0.62	0.02	0.49	0.33	0.04
Example 3						
$q = 0$	0.26	0.41	0.21	0.27	0.42	0.22
$q = 1$	0.52	0.52	0.14	0.36	0.36	0.15
$q = 2$	0.80	0.67	0.08	0.33	0.20	0.10

Notes: Example 1 represents completely distinct lineages, with 10 species in each assemblage and no shared species. Example 2 has 23 species in Assemblage 1, 19 species in Assemblage 2; and 5 shared species. Example 3 contains rockfish data, with 38 species in Assemblage 1, 24 species in Assemblage 2, and 23 shared species. See Tables 1 and 2 and Eq. 13a for formulas. Note the small difference between the classical phylogenetic measure $J_{qN}(T)$ and its corresponding non-phylogenetic measure J^*_{qN} for all cases. These two additive "beta"/gamma measures cease to reflect either tree structure or differences in species abundances, so they should not be used. For Example 1, phylogenetic and corresponding non-phylogenetic measures are identical because species are equally distinct.

assemblages over this time interval. In contrast, the traditional differentiation measure $J_{qN}(T)$ (based on phylogenetic generalized entropies, Eq. 13a) depends on the richnesses S of the assemblages. Table 3 shows the $J_{qN}(T)$ measures for the special case of $S = 10$. As derived in Appendix F, the general formula is $J_{2N}(T) = 1/(2S - 1)$, while $J_{1N}(T) = (\log 2)/\log(2S)$, and $J_{0N}(T) = S/(2S - 1)$. This means that when the alpha diversity is large (equivalently S is large for this example), both J_{2N} and J_{1N} always approach zero, wrongly indicating that there is almost no differentiation. The measure J_{0N} approaches 1/2, indicating a normalization is needed. For this example, the correct answer is unequivocal: The two completely phylogenetically distinct assemblages should attain the maximum differentiation of unity. The traditional measures cannot measure differentiation properly even for a simple tree, so they cannot do it for a more complicated tree either.

Example 2: A more complex hypothetical tree

We now consider a more complicated hypothetical tree in order to examine the performance of differentiation measures as a function of evolutionary time. Consider a homogeneous super-continent that splits into two continents or assemblages. Fig. 3 shows the time-calibrated phylogenetic tree of the fauna of these continents. We assume that the age of the basal node is 240 million years (Myr) ago. The continental split occurs at 200 Myr ago (i.e., $t = 40$ Myr after the first node). While the continents are still joined, their faunas are identical with five taxa. Suppose the taxa vary in their dispersal abilities. Then, after separation, some taxa radiate independently on each of the new continents, while others continue to cross the gap and are shared between continents. Assume that in the two present-day assemblages, there are 23 species in Assemblage 1 and 19 species in Assemblage 2, with 5 of these shared between assemblages (Fig. 3). We focus on the differentiation measure with equal weights in order to compare our measures with the additive approach. In each assemblage, all species are assumed to be equally abundant at the present time, and the actual relative abundances of the ancestral species in the past are the sums of the relative abundances of their descendants in the present-day assemblages. If an approach fails in this simple case, it cannot be a mathematically valid approach for more realistic cases.

Table 3 compares the non-phylogenetic and phylogenetic differentiation measures when the temporal perspective T is chosen to be the age of the basal node, 240 Myr ago. The phylogenetic measure $J_{qN}(T)$ hardly differs from its non-phylogenetic counterpart J^*_{qN}. In contrast, the difference between our new phylogenetic measures and their non-phylogenetic counterparts depends on q. The difference is limited for $q = 0$, but the difference for $q > 0$ can be substantial.

Now imagine that we have been monitoring these assemblages since $T = -240$ Myr, and we watch how the assemblages diverge over time. If we are using sensible measures of evolutionary differentiation, we should witness the divergence increasing monotonically with time. We test this by plotting the temporal evolution of various differentiation measures beginning at the first node, as a function of time t after the first node. That is,

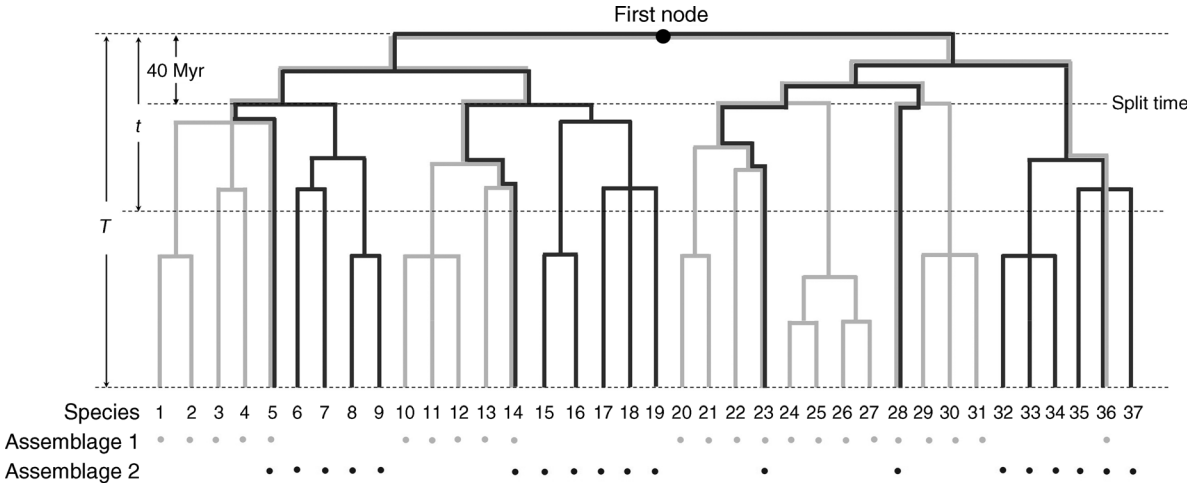

FIG. 3. A hypothetical time-calibrated tree with the age of the first node $T = 240$ million years ago (Myr). The split occurs at an age of 200 Myr ago (i.e., 40 Myr after the first node). At the present-day assemblage, there are 23 species in assemblage 1 (gray), and 19 species in assemblage 2 (black), and there are five shared species. In each assemblage, all species are assumed to be equally abundant at the present time for illustrative purposes. When a differentiation measure is computed for the interval $[-T, -T + t]$ as a function of t, the variable t denotes the time after the age of the root, $0 \leq t \leq 240$. The spilt time corresponds to a specific value of $t = 40$.

we graph the differentiation measure between the two assemblages for the interval $[-T, -T + t]$, as a function of t, with t ranging from zero (the basal node) to 240 Myr. A measure of normalized phylogenetic differentiation should be low (and zero for $q = 0$) when applied to the assemblages for $t < 40$ Myr, because this is the period when the species are all shared by the two assemblages prior to the continental break-up. Phylogenetic differentiation should increase monotonically beginning immediately after the break-up at $t = 40$ Myr, since the assemblages evolve independently after this time, diverging due to genetic drift and the action of different selective forces. After a very long time, the normalized differentiation should eventually approach unity.

In this example, all measures are computed for the interval $[-T, -T + t]$ as a function of t instead of the time perspective T, so we drop the variable T in all notations of measures. The graphs in Fig. 4 demonstrate the behavior of the traditional differentiation measure J_{qN} and our two phylogenetic differentiation measure $1 - \bar{C}_{qN}$ and $1 - \bar{U}_{qN}$ for $q = 0$, 1, 2. When $q = 1$, the two measures $1 - \bar{C}_{1N}$ and $1 - \bar{U}_{1N}$ are identical; for $q = 0$, the measure $1 - \bar{U}_{0N}$ is higher than $1 - \bar{C}_{0N}$ while the ordering is reversed for $q = 2$. From Fig. 4, it is clear that our phylogenetic differentiation measures behave as expected and generally exhibit a consistent trend. They are both low (and zero for $q = 0$) prior to the break-up of the continents, and increase monotonically afterwards. The asymptotic values of our two normalized differentiation measures approach unity, although for $q = 2$, the rates of increase are slow.

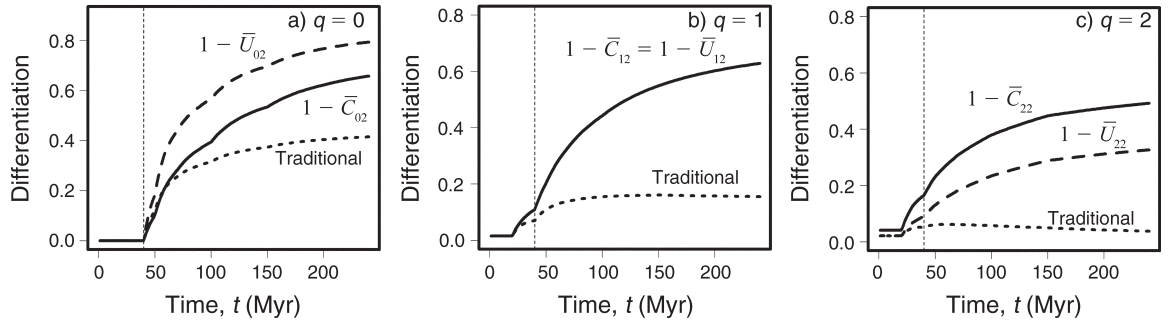

FIG. 4. Plot of differentiation for the traditional additive phylogenetic differentiation measure J_{qN} (based on phylogenetic generalized entropies) and our proposed phylogenetic differentiation measures $1 - \bar{C}_{qN}$ and $1 - \bar{U}_{qN}$ (both are based on our mean phylogenetic diversity). See Eq. 11a for the definition of $\bar{C}_{qN}$, and Eq. 12a for the definition of $\bar{U}_{qN}$, but all measures are computed for the interval $[-T, -T + t]$ and plotted as a function of time t after the root for (a) $q = 0$, (b) $q = 1$, and (c) $q = 2$. Here T is fixed to be 240 Myr, the age of the first node. The vertical dotted line refers to the split time ($t = 40$ Myr after the first node). See Appendix G for the profiles of the three differentiation measures as a function of the time perspective T when all measures are computed for the interval $[-T, 0]$.

For $q = 0$, the measure J_{0N} displays a pattern similar to that of our measures; after the split, it steadily increases to a stable value, but it stabilizes at a different value than our measures. In sharp contrast, the traditional differentiation measures based on phylogenetic entropy ($q = 1$) and quadratic entropy ($q = 2$) in Fig. 4 begin to *decrease* after an initial rise following the continental break-up. For both, the asymptotic value is very low rather than unity. These measures will therefore mis-rank assemblages according to their phylogenetic differentiation. For example, the assemblages 200 Myr after the split are unambiguously more differentiated than the assemblages just 20 Myr after the split, but the traditional differentiation measures for $q = 1$ and $q = 2$ give the opposite ranking. These misbehaviors are consequences of their dependence on alpha, as predicted by our Eqs. 13b, 13c, and 13d. All these behaviors are analogous to the corresponding behaviors of non-phylogenetic "similarity" and "differentiation" measures based on classical indices like Shannon entropy and the Gini-Simpson index, as shown in Figs. 1 and 2 of Jost et al. (2010).

In this example, all the differentiation measures are computed for the interval $[-T, -T + t]$, where T is fixed value of 240 Myr (the age of the root). This is because the plot as a function of t (time after the age of the root) should unequivocally exhibit a non-decreasing trend so we can examine whether a measure behaves as expected. As discussed, we recommend in most applications to present two types of profiles to see how our proposed differentiation measures $1 - \bar{C}_{qN}(T)$ and $1 - \bar{U}_{qN}(T)$ behave when the temporal perspective T varies (for a fixed q) or when order q varies (for a fixed T). These two types of profiles for the hypothetical tree are shown in Appendix G. These two types of profiles are illustrated for a real phylogenetic tree in Example 3 with discussion.

Example 3: A real phylogenetic tree for rockfish

We now apply our methods to a real example discussed by Pavoine et al. (2009). The full data set contains a total of 52 rockfish species of the genus *Sebastes* collected over 20 years (1980–1986, 1993–1994, 1996, 1998–2007) from the Southern California Bight, USA. Love et al. (1998) found that the species richness declined at a constant rate due to heavy fishing in recent decades. Considering phylogeny, Magnuson-Ford et al. (2009) concluded that the large, evolutionarily isolated and morphologically distinctive species generally are more vulnerable to overfishing. Pavoine et al. (2009) applied their phylogenetic generalized entropy, given in our Eq. 2c, to examine whether the decline in species richness was associated with the change in the phylogenetic structure of the assemblage.

For illustrative purposes, we focus on measuring the phylogenetic differentiation between two contrasting assemblages. (Some additional analyses are provided in Appendix G.) The 1981 and 2003 assemblages are referred to as Assemblage 1 and 2, respectively. The phylogenetic tree of the 52 species (from Hyde and Vetter 2007) and the species relative abundances for these two assemblages, taken from Pavoine et al. (2009), are shown in Fig. 5a. Our purpose is to quantify the phylogenetic differentiation among the two sets of relative abundances, the weights for the two assemblages are thus equal in our analysis. A sub-tree containing only the three most abundant species in each assemblage is shown in Fig. 5b.

Consider a fixed time perspective at $T = 7.9$ Myr, the age of the root of the pooled tree. All the phylogenetic and non-phylogenetic differentiation measures for the interval $[-7.9, 0]$ are presented in Table 3. As we found for Example 2, the traditional abundance-sensitive differentiation measures $J_{qN}(T)$ ($q > 0$) are very low and close to their non-phylogenetic value J^*_{qN}. Both our phylogenetic differentiation measures, $1 - \bar{C}_{qN}(T)$ and $1 - \bar{U}_{qN}(T)$, are greater than or equal to the additive measure for all orders of q, especially for $q = 2$. These relations will be explained in the rest of this section.

As we did with the hypothetical tree of Fig. 4, we compute the traditional measure J_{qN} and the two differentiation measure $1 - \bar{C}_{qN}$ and $1 - \bar{U}_{qN}$ for the interval $[-T, -T + t]$. In Fig. 6, we plot the three differentiation measures as a function of time t (time after the root). The plots in Fig. 6 (analogous to the plots in Fig. 4 for the hypothetical tree) show that, for $q = 0$, the three measures all exhibit similar pattern and stabilize, but for $q = 1$ and 2, the patterns of our measures are very different from that of J_{qN}, as we also saw in Fig. 4. For $q = 1$ and 2, the three measures all start to rise sharply at 1.6 Myr after the root, roughly the time that the most abundant species *S. miniatus* in Assemblage 2 diverged from the lineage of the three most abundant species in Assemblage 1 (*S. paucispinis*, *S. goodei*, *S. mystinus*); see Fig. 5b. After 1.6 Myr, our measures $1 - \bar{C}_{qN}$ and $1 - \bar{U}_{qN}$ steadily increase with time to a relatively high value, while the traditional measure J_{qN} decreases (especially for quadratic entropy) to a relatively low value. Once again, we are seeing the effect of the inequality given in Eqs. 13b, 13c, and 13d; these traditional "differentiation" measures will always tend to zero whenever gamma is high for $q = 1$, and whenever alpha is high for $q = 2$; they cease to reflect either tree structure or differences in species abundances.

These discrepancies are similar to our findings for the hypothetical tree in Fig. 4, where it is clear that the more reasonable answer is given by our measure. In this real example, the increasing trend and high differentiation shown by our measures should also be the more intuitive and sensible answer after 1.6 Myr. Consider first the non-phylogenetic differentiation measure for $q = 2$. The two measures $1 - C_{2N}$ and $1 - U_{2N}$ both are dominated by the relatively common species shown in Fig. 5b. The most common species in Assemblage 1 correspond to a very rare species in Assemblage 2, and vice versa; see Fig. 5b. Therefore, when phylogeny is not considered,

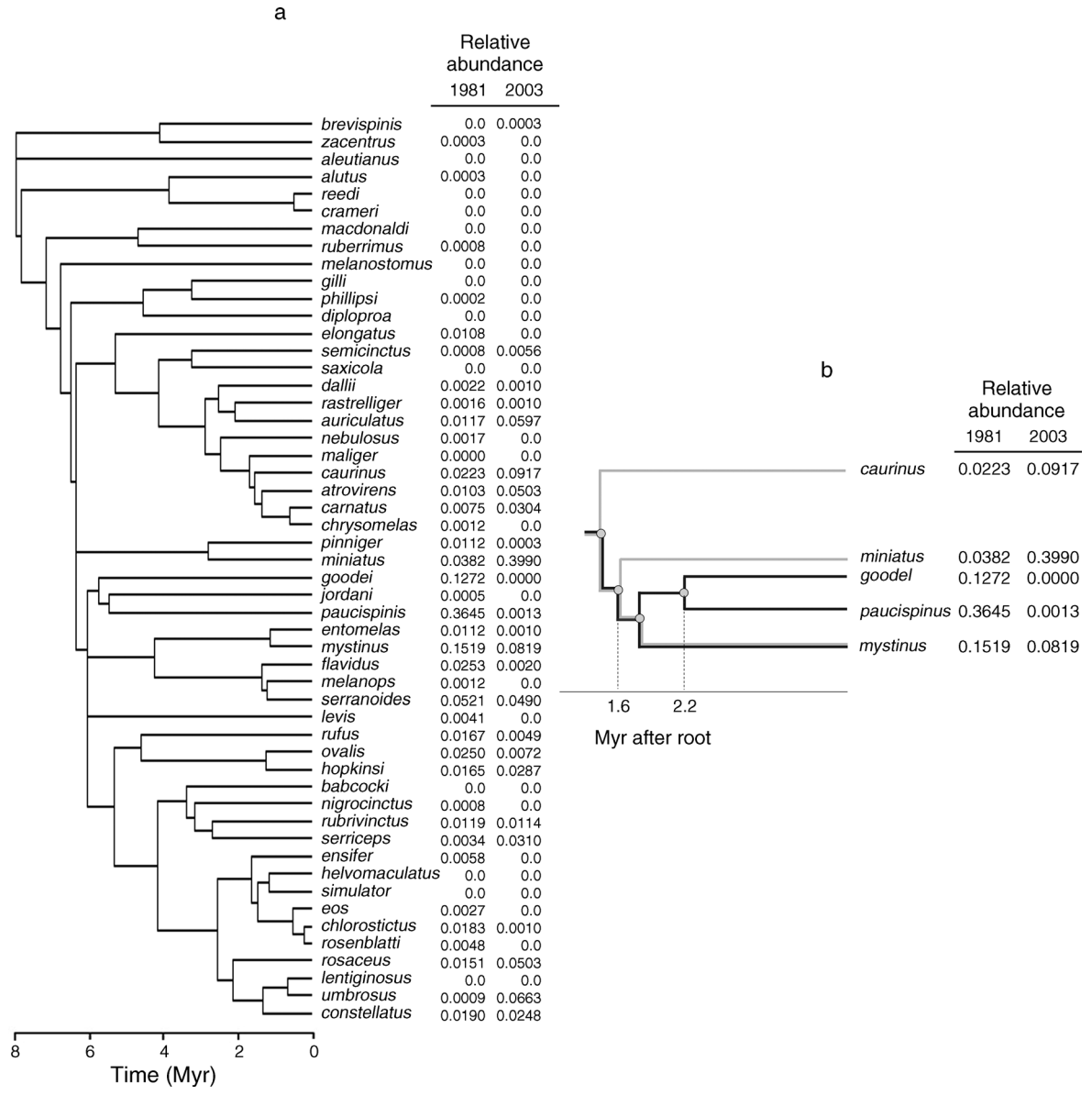

FIG. 5. (a) The phylogenetic tree of 52 rockfish species of the genus *Sebastes* (Hyde and Vetter 2007) and the relative abundances (proportions) for 1981 and 2003 (Pavoine et al. 2009). The age of the root is $T = 7.9$ Myr. (b) A sub-tree contains only the three most abundant species in each assemblage (those with relative abundance >8%). The phylogenetic tree for the three most abundant species in assemblage 1 is in black, and the phylogenetic tree for the three most abundant species in assemblage 2 is in gray.

the differentiation should be relatively high, as reflected by the high value of $1 - C_{2N} = 80\%$ and $1 - U_{2N} = 67\%$ at the tips (present day) in Table 3. The former is the effective average percentage of dominant species that are unique to each assemblage (and thus shared species constitute only about 20% of the dominant species in each assemblage). The latter is the effective percentage of dominant species that are unique to the pooled assemblage (and thus, shared species constitute about 33% of the dominant species in the pooled assemblage).

Our phylogenetic differentiation measures $1 - \bar{C}_{2N}$ and $1 - \bar{U}_{2N}$ are dominated by the "very important lineages" (those with high node abundances) and "evolutionarily deep" species (long branch lengths). The most dominant species of Assemblage 2 (*S. miniatus*) diverged from the lineage of the three dominant species in Assemblage 1 around 1.6 Myr after the root; see Fig. 5b. The divergence time for the three most dominant species of Assemblage 1 occurred between 1.6 Myr and 2.2 Myr after the root. Around 2.2 Myr after the root, all five dominant species in Fig. 5b are in isolated lineages, and the sharp importance difference between the dominant ancestral lineages remains after that. Thus, the phylogenetic differentiation

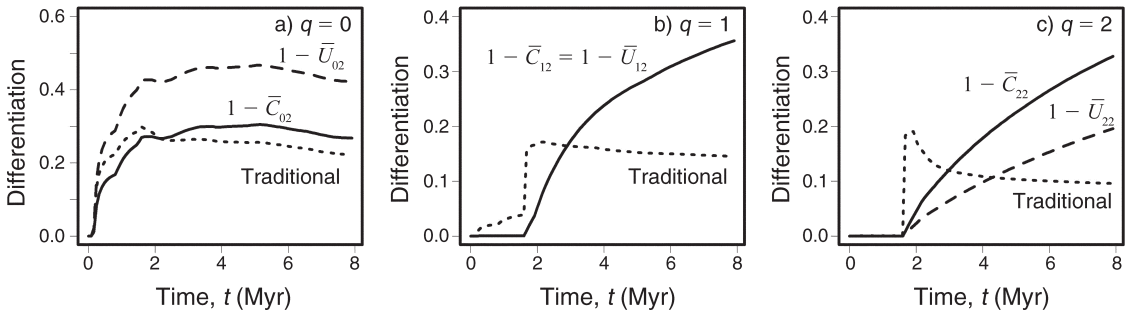

FIG. 6. Plot of differentiation between two rockfish assemblages for the traditional additive phylogenetic differentiation measure J_{qN} (based on phylogenetic generalized entropies) and our proposed phylogenetic differentiation measures $1 - \bar{C}_{qN}$ and $1 - \bar{U}_{qN}$ (both are based on our mean phylogenetic diversity). All measures are computed for the interval $[-T, -T + t]$ and plotted as a function of time t after the root for (a) $q = 0$, (b), $q = 1$, and (c) $q = 2$.

between these two assemblages should begin increasing at 1.6 Myr after the root and should continue to increase with time t.

Our phylogenetic differentiation measure $1 - \bar{C}_{2N}$ increases to 33% by the present time (Table 3 and the right panel of Fig. 6 as t approaches 7.9 Myr). Similarly, the measure $1 - \bar{U}_{2N}$ increases to 20%. These are substantially lower than their corresponding non-phylogenetic differentiation measure because the node abundances near roots (where the differentiation values are near zero) are relatively high and dominant in the whole tree. But these values are much higher than the traditional additive phylogenetic "differentiation" values; our value for $q = 2$ is triple the value of 10% based on Rao's quadratic entropy. In the past 7.9 Myr, if we focus on the abundant lineages (as appropriate for $q = 2$), the average percentage of non-shared lineages per assemblage is about 33% (and 20% in the pooled assemblage), showing that the values of our measures (33% and 20%) reflect reality, while the traditional additive measure may underestimate the phylogenetic effects of overfishing. Similarly for $q = 1$, the differentiation for our measure ($1 - \bar{C}_{1N} = 1 - \bar{U}_{1N}$) increases from zero to 36%, whereas the corresponding curve for phylogenetic entropy rises briefly and then counterintuitively drops to a low value of around 15% (Table 3, Fig. 6).

To see how our differentiation measures vary with the time perspective T and with the order q, we suggest making two types of profiles for our proposed differentiation measures. The first type of profile plots the differentiation measure as a function of the temporal perspective T, with q fixed. The second type plots the same measure as a function of q, with T fixed. To illustrate the first type of profile, we evaluate the two proposed differentiation measures, $1 - \bar{C}_{qN}(T)$ and $1 - \bar{U}_{qN}(T)$, over the interval $[-T, 0]$ with $0 < T < 10$, for q fixed; in Fig. 7a we choose to plot the profiles for $q = 0$, 1, and 2. For comparison, we also plot the profiles of the traditional measure $J_{qN}(T)$ for the same fixed values of q. In Fig. 7b, we show the other type of profiles, which plot the three measures as a function of q, $0 \leq q \leq 5$, separately for $T = 0$ (non-phylogenetic case) and $T = 7.9$ Myr.

The profiles in Fig. 7a show that the additive differentiation measure $J_{qN}(T)$ hardly varies with T, and all values for $q = 1$ and $q = 2$ are very low, as predicted by our theory for the case of high alpha (and thus high gamma) phylogenetic entropies. In such cases, the measure $J_{qN}(T)$ is nearly insensitive to the phylogenetic structure. This can also be seen by comparing the two profiles in Fig. 7b for the specific values of $T = 0$ (non-phylogenetic cases) and $T = 7.9$ Myr for $0 \leq q \leq 5$. All values of the measure $J_{qN}(T)$ for $T = 7.9$ Myr are close to their corresponding non-phylogenetic values for $T = 0$ (i.e., the measure J^*_{qN}); see also Table 3. The two measures $J_{qN}(T)$ and J^*_{qN} vary slowly with the order q as shown in Fig. 7b, and their values are very low (for $q \geq 1$) as predicted by our theory. Therefore, the two types of profiles in Figs. 7a and 7b confirm by example our theoretical proof that the measure $J_{qN}(T)$ often will not reflect either tree structure or differences in species abundances.

We next examine the behavior of our two proposed differentiation measures. Since the dominant species in the two assemblages began to diverge from each other between 1.6 Myr and 2.2 Myr after the root (i.e., between 5.7 Myr ago and 6.3 Myr ago; see Fig. 5b), those dominant species were in the same lineage 6.3 Myr ago or anytime earlier. As a result, the two proposed abundance-sensitive measures ($q = 1$ and 2) in Fig. 7a remain at relatively high levels when $T < 6.3$ Myr and start to decline around $T = 6.3$ Myr. Generally, as T becomes larger, more dominant shared lineages are added to the two assemblages, implying the abundance-sensitive differentiation measures should generally exhibit a nonincreasing trend. The profiles of our differentiation measures for $q = 1$ and 2 clearly show the expected decreasing trend when T is increased, and the decline rates differ for the two different orders of q. Also, comparing the two figures ($T = 0$ and $T = 7.9$ Myr) in Fig. 7b, we see that all values of the phylogenetic

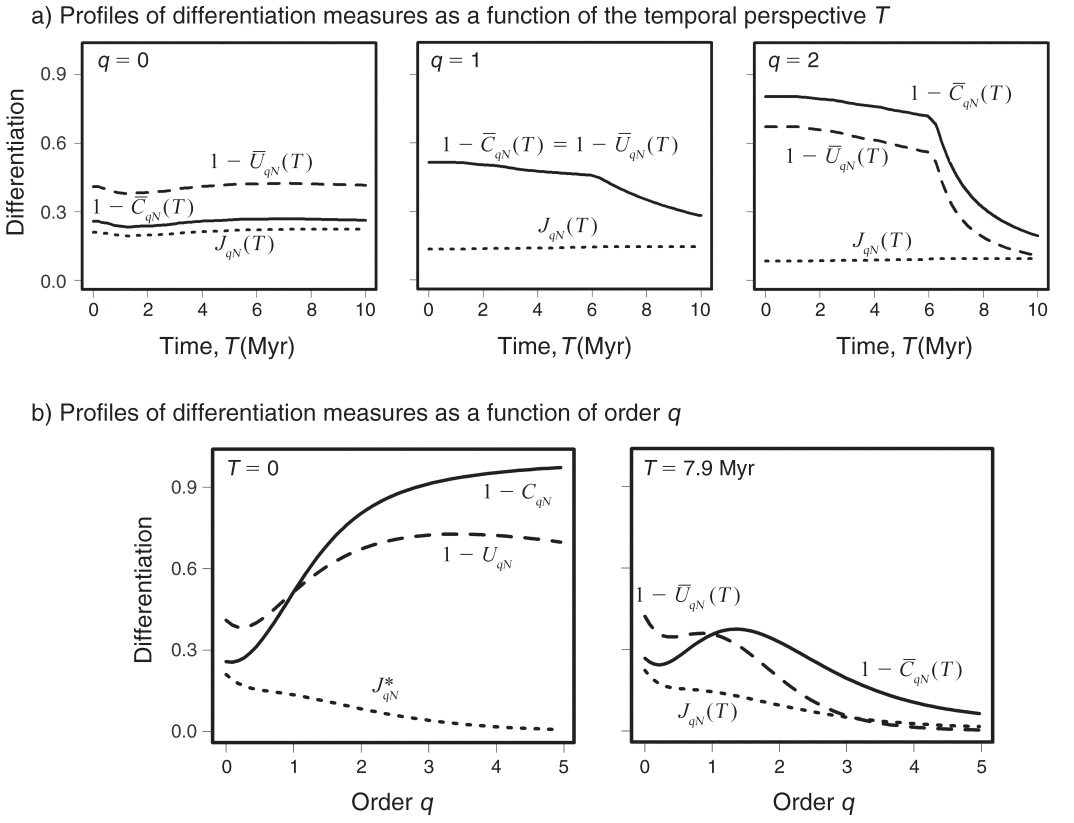

FIG. 7. Profiles of differentiation measures. (a) Profiles of the two proposed phylogenetic differentiation measures, $1 - \bar{C}_{qN}(T)$ and $1 - \bar{U}_{qN}(T)$, and the traditional measure $J_{qN}(T)$, as a function of the time perspective T for $q = 0$, $q = 1$, and $q = 2$, $0 \leq T \leq 10$. All measures are computed for the interval for the interval $[-T, 0]$, where T varies from 0 to 10. (b) Profiles of the corresponding non-phylogenetic differentiation measures (i.e., $T = 0$), $1 - C_{qN}$, $1 - U_{qN}$ and J^*_{qN}, as a function of order q, $0 \leq q \leq 5$. Profiles of the three phylogenetic differentiation measures, $1 - \bar{C}_{qN}(T)$, $1 - \bar{U}_{qN}(T)$, and $J_{qN}(T)$, as a function of order q, $0 \leq q \leq 5$, for the specific time perspective $T = 7.9$ Myr, the age of the root of the pooled phylogenetic tree.

differentiation measure $1 - \bar{C}_{qN}(T)$ are much lower than the corresponding non-phylogenetic measure. Similar behavior is also found for the measure $1 - \bar{U}_{qN}(T)$. The two types of profiles (in Fig. 7a and b) show that our measures can incorporate the differences in both tree structure and lineage abundances.

These hypothetical and real examples have confirmed empirically our theoretical findings in earlier sections. If our goal is to provide measures to quantify the similarity or differentiation, and compare the measures across regions with different alpha or gamma diversities, the traditional additive "differentiation" measures based on (1 − alpha/gamma) for phylogenetic entropy and quadratic entropy may lead to counterintuitive results, and for $q > 0$, they are insensitive to tree structure when alpha diversity is high. For all orders of q, these traditional measures can be fixed by normalizing them, again yielding our differentiation measures $1 - \bar{C}_{qN}$ and $1 - \bar{U}_{qN}$, whose ranges are always the interval [0, 1] regardless of alpha or gamma diversity. Our measures behave as expected and conform to intuition, as shown by all examples.

DISCUSSION

In the past, a traditional additive approach has been applied to partitioning phylogenetic measures such as Rao's quadratic entropy Q, phylogenetic entropy H_P, and phylogenetic generalized entropy. The difference between gamma and alpha phylogenetic generalized entropies (which include quadratic entropy and phylogenetic entropy as special cases) was then divided by gamma to obtain measures of phylogenetic differentiation. While these measures do have valid interpretations (Hardy and Jost 2008), their magnitudes do not reflect the degree of phylogenetic differentiation between assemblages. Our examples and mathematical analyses show that when within-group diversity is high, these abundance-sensitive differentiation measures approach a fixed value (zero) that has no relation to the phylogenies of the species or to the differences in their abundances across assemblages. Measures that become completely insensitive to the properties they are supposed to measure are not useful tools for biologists, and they will inevitably mislead in typical conservation and applications.

This behavior, caused by the measures' dependence on alpha diversity, has other disturbing consequences. The additive differentiation measure based on Rao's quadratic entropy can show that every single subfamily of plants exhibits very high differentiation (no shared lineages) between two assemblages, but when the same measure is applied to the pooled subfamilies, it would show that differentiation between the two assemblages was near zero. This can happen even if all subfamilies shared the same root node and had the same tree structure and same abundance distributions. The mere act of pooling necessarily lowers this differentiation measure, because pooling equally diverse subfamilies makes alpha increase, and this measure is confounded with alpha. These problems have clear mathematical causes. First, the additive framework was imposed on measures that are not additive (except when $q = 1$), resulting in a between-group component that is confounded with the within-group component. Second, the measures do not obey the replication principle, so their alpha/gamma ratio does not reflect similarity between groups.

These are familiar problems that also arise when the additive framework is applied to non-phylogenetic generalized entropies. In the non-phylogenetic case, these problems were resolved by partitioning Hill numbers, which obey the replication principle (Jost 2007). In this paper we show how to extend this solution to the phylogenetic case, by partitioning the phylogenetic Hill numbers of Chao et al. (2010). Phylogenetic Hill numbers are multiplicatively partitioned into independent within- and between-group components, which are the phylogenetic alpha and beta diversities. The between-group or beta component is normalized in various ways to make phylogenetic similarity and differentiation measures. The normalizations yield weighted and phylogenetic generalizations of the Jaccard, Sørensen, Horn, and Morisita-Horn similarity measures. The proposed normalized similarity measures have the flexibility to reflect the resemblance or difference not only in relative abundances, but also in absolute abundances.

As in the non-phylogenetic case, the lineage excess (gamma − alpha phylogenetic Hill numbers) and the phylogenetic generalized entropy excess (gamma − alpha phylogenetic generalized entropies), when normalized properly, lead to some of these same similarity measures. The convergence of all these approaches demonstrates the underlying unity of this field and highlights the special character of our similarity measures $\bar{C}_{qN}(T)$ and $\bar{U}_{qN}(T)$; see Table 2. The similarity measure $\bar{C}_{qN}(T)$ quantifies the effective average proportion of shared lineages per assemblage. The differentiation measure $1 - \bar{C}_{qN}(T)$ thus quantifies the effective average proportion of non-shared lineages per assemblage. The measure $\bar{C}_{qN}(T)$ satisfies a phylogenetic generalization of the concept of a "true local overlap" measure (Wolda 1981, 1983). This quality "calibrates" the similarity measure in terms of an easily-visualizable set of reference assemblages. A similar interpretation can be made for the regional-overlap similarity measure $\bar{U}_{qN}(T)$, which refers to the effective percentage of shared lineages in the pooled assemblage.

All similarity and differentiation measures that are monotonic transformations of our phylogenetic beta diversity (see Table 2) are replication invariant. For non-phylogenetic measures, this principle states that if N assemblages each consist of K identical subsets of abundances, and no species are shared between subsets within an assemblage, then the N assemblages as a whole should have the same degree of similarity or differentiation as the individual subsets. Jost et al. (2011) showed that this property is a necessary property for classical non-phylogenetic similarity and differentiation measures. Our proposed phylogenetic beta, similarity, and differentiation measures all satisfy this property of replication invariance; see Appendix C for a proof. This means our measures, unlike previous ones, are self-consistent when disjoint sub-trees are pooled.

Choice of temporal perspective T and order q

A conspicuous change from previous treatments of phylogenetic differentiation measures is our introduction of an explicit parameter T for the temporal perspective of the investigator. We introduced this in Chao et al. (2010), but it is even more important here. The broader our temporal perspective, the greater is the proportion of shared ancestry in the assemblages. Measures of normalized phylogenetic similarity have always concealed an implicit temporal perspective, most often the age of the root node of the tree under consideration. However, this choice is not always the most appropriate one for the question under investigation. One problem with this choice is that it is sample dependent, because the root will be determined by the species actually observed. Since nearly every study will use a different root, it will be difficult to compare results across studies. By making the perspective explicit, we give the investigator the freedom to think about this choice and, if necessary, to change it. The most natural and least arbitrary choice of temporal perspective T for many purposes will be the divergence time between the group of interest and its nearest outgroup. This is independent of the composition of the actual sample and depends only on the sampling protocol (the decision to sample members of one taxonomic group, birds for example, and reject others such as moths or bats). Another natural choice would be T near the time of the most recent common ancestor of all taxa alive today. Other choices may be useful depending on the purpose of an investigation. Because different investigations will require different temporal perspectives, we recommend reporting results in a form that facilitates changes of this perspective. Reporting ${}^{q}\bar{D}(T_r)$, with T_r equal to the age of the root node for the organisms under study, allows easy transformation to any time interval larger than T_r.

If T is the new temporal perspective, then

$$ {}^{q}\bar{D}(T) = \left\{ \frac{T - T_r}{T} + \frac{T_r}{T} [{}^{q}\bar{D}(T_r)]^{1-q} \right\}^{1/(1-q)}. $$

This formula can be used to translate both phylogenetic alpha and gamma diversity to the new temporal perspective. The new alpha and gamma diversities can then be used to calculate beta and our similarity (or differentiation) measures for the new T. See Fig. G1 (in Appendix G) and Fig. 7a for examples of profiles for our proposed phylogenetic differentiation between two assemblages as a function of the time perspective T.

Our measures also contain the free parameter q, which determines the sensitivity to present-day species abundances. When trying to identify past episodes of differentiation, $q = 0$ is recommended, since abundance information is not necessarily relevant to this question. In ecological studies such as those examining the phylogenetic relationships of the dominant species in a set of assemblages, or those examining functional diversity, we recommend reporting the results in the form of a similarity or differentiation profile, a graph of the chosen measure(s) as q varies from zero to about four or five (beyond which there is usually little change). This gives complete information about the system for the chosen time perspective T, just as in the non-phylogenetic case; see Jost et al. (2011) for a non-phylogenetic similarity profile, and Fig. G1 (in Appendix G) and Fig. 7b for phylogenetic differentiation profiles of our proposed measures, as functions of q.

Functional beta diversity

Functional diversity (FD) has been defined by Tilman (2001) as "the value and range of those species and organismal traits that influence ecosystem functioning." Many measures have been proposed to assess FD of an assemblage. Among them, the dendrogram constructed from a trait-based distance matrix using a clustering scheme (Petchey and Gaston 2002) is widely used. Chao et al. (2010) suggested that the phylogenetic mean diversity approach given in Eqs. 4a and 4b can be applied to quantify functional diversity and interpreted as "the effective mean number of functional groups." The approach proposed in the present paper can be used to quantify functional beta diversity among assemblages, and to generate intuitive and well-behaved measures of functional similarity and differentiation among assemblages. The partitioning method can also provide a unified framework for genetic, species, and ecosystem diversity partitioning. A critical requirement in our approach is that a tree structure can be constructed. We are currently developing Hill number types of functional diversity based on distance matrix directly.

Applications to other disciplines

The concept of diversity and its partitioning are useful in many disciplines. Our proposed decomposition can be applied in these disciplines, especially genetics. For example, a widely used genetic "differentiation" measure is Nei's G_{ST} based on heterozygosity, the Gini-Simpson index of ecologists (Nei 1973, Jost 2008). ($G_{ST} = 1 - H_{GS,\alpha}/H_{GS,\gamma}$ where $H_{GS,\gamma}$ and $H_{GS,\alpha}$ denote, respectively, gamma and alpha Gini-Simpson index.) It is often used to measure the differentiation of allele frequencies among subpopulations. Jost (2008) showed that G_{ST} and their relatives do not actually measure differentiation and proposed a new differentiation measure D, which is our $1 - C_{2N}$ measure (Table 1). Our new phylogenetic differentiation measure $1 - \bar{C}_{2N}(\bar{T})$ (Eqs. 11b and 11c) generalizes Jost's D to take into account genetic distances and assemblage weights. For this purpose, geneticists have often used the differentiation measure N_{ST} (Nei and Li 1979), which is based on nucleotide diversity (the average number of nucleotide differences between any two DNA sequences chosen randomly from a population). ($N_{ST} = 1 - Q_\alpha/Q_\gamma$ where Q_γ and Q_α denote, respectively, gamma and alpha quadratic entropy.) The nucleotide diversity is equivalent to Rao's quadratic entropy, and N_{ST} is identical to the traditional differentiation measure $J_{2N}(T)$. We have shown here by hypothetical and real examples that the measure $J_{2N}(T)$ based on additive partitioning of Rao's quadratic entropy does not measure differentiation. Thus, N_{ST} suffers the same drawback as G_{ST} and the measure $J_{2N}(T)$. However, like additive beta quadratic entropy, it can be easily corrected, and the corrected measure is exactly our proposed phylogenetic differentiation measure $1 - \bar{C}_{2N}(\bar{T})$, the phylogenetic generalization of Jost's D measure; see Eq. 11b. This generalized measure is valid for both ultrametric and non-ultrametric trees. Hence, it also extends de Bello et al. (2010) to the general non-ultrametric weighted case. This provides a unified and rigorous framework for quantifying pure phylogenetic differentiation in both ecology and genetics, without confounding differentiation with within-group phylogenetic diversity. The new differentiation measure $1 - \bar{U}_{2N}(\bar{T})$ merits investigation of its applications to genetics.

Leinster and Cobbold (2012) wrote "non-specialists are amazed to learn that a community of six dramatically different species is said to be no more diverse than a community of six species of barnacle." Now that phylogenetic versions of the full range of diversity, similarity, and differentiation measures are available, it makes sense to incorporate phylogeny in all future diversity analyses. We hope that these new tools will encourage ecologists, geneticists, and conservation biologists to ask and answer new kinds of questions about the evolutionary forces that cause divergence of species assemblages or gene pools.

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Supplemental Material

Appendix A

An illustrative ultrametric tree (*Ecological Archives* M084-002-A1).

Appendix B

Diversity profile and strong replication principle for Hill numbers and phylogenetic Hill numbers (*Ecological Archives* M084-002-A2).

Appendix C

Diversity decomposition and related properties (*Ecological Archives* M084-002-A3).

Appendix D

Derivation of four classes of similarity measures and related properties (*Ecological Archives* M084-002-A4).

Appendix E

Mathematical flaws in the traditional additive approach based on generalized entropy excess or phylogenetic generalized entropy excess (*Ecological Archives* M084-002-A5).

Appendix F

A simple hypothetical tree with completely distinct lineages (*Ecological Archives* M084-002-A6).

Appendix G

Additional analysis of Examples 2 and 3 (*Ecological Archives* M084-002-A7).

Data Availability

Data associated with this paper have been deposited in Dryad: http://dx.doi.org/10.5061/dryad.vr4k2