

## **SUPPLEMENTAL APPENDIX 1: COMPARISONS WITH OTHER UNIFIED MEASURES**

This Supplemental Appendix is a slightly modified version of appendix S5 of Chiu & Chao (2014).

### **1. LEINSTER AND COBBOLD MEASURE**

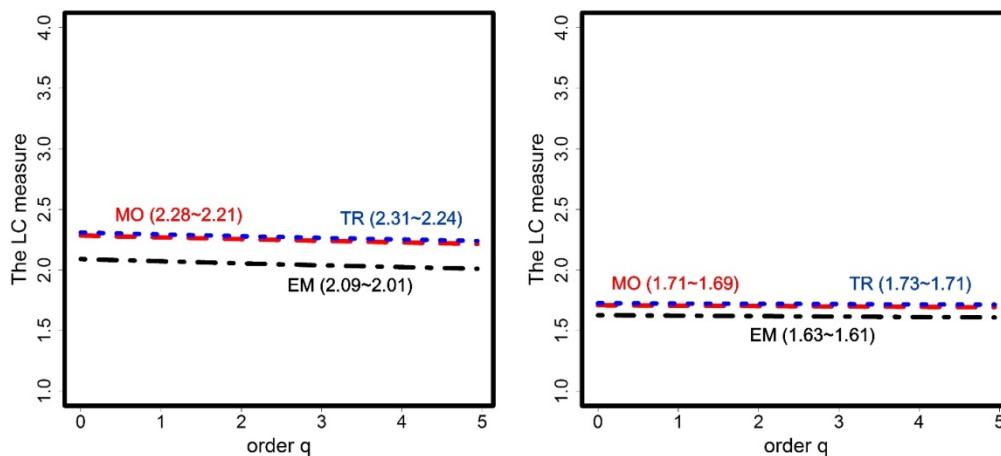
Leinster & Cobbold (2012) derived a parametric class of measures sensitive to species similarity based on a framework of Hill numbers. We find that their measure (hereafter referred to as the LC measure) may not be sensitive to species abundances if the species similarity matrix is computed from species traits in functional analysis. When a species similarity matrix deviates greatly from a naive identity matrix, their measure typically yields very low diversity values, especially for assemblages with many species; this causes problems for the interpretation of “species equivalents” in their approach. Note that, in the bottom right panel of figure 3 of Leinster & Cobbold (2012), as  $q$  varies between 0 and 5, their measure for a non-naive similarity matrix decreases from 1.27 to 1.25 for case “TS1” with roughly 250 species and, as shown in the bottom left panel of their figure 3, decreases from 1.25 to 1.22 for case “TS3” with roughly 200 species. This reveals that the LC measure hardly varies with the order  $q$  for the two cases considered in their figure 3. We thus computed several other real examples to see whether the LC measure generally exhibits a similar pattern. We describe one typical example to show our findings.

We applied the LC measure to the real data discussed in Ricotta et al. (2012). The same data were also analyzed in Chiu & Chao (2014). We apply our own measures to these data in

[Supplemental Appendix 5](#) of the present paper, so that readers can make comparisons. The full

data contain a total of 43 vascular plant species collected from 272 random vegetation plots of  $2 \times 2$  m in size during the period 2002–2009 in three fore-dune habitats: embryo dunes (EM) (17 species in 70 plots), mobile dunes (MO) (39 species in 131 plots), and transition dunes (TR) (42 species in 71 plots) along the Tyrrhenian coast (for details, see Carboni et al. 2010, 2011, 2013). In each habitat, we pooled species abundances over plots and obtained species relative abundances (see **Supplemental Figure 2** in [Supplemental Appendix 5](#)).

All species were described by a set of 16 functional traits. On the basis of these 16 traits, the species distance matrix was calculated by a Gower mixed-variables coefficient of distance (Pavoine et al. 2009). Because Gower's distance between any two species is between 0 and 1, the one complement of each distance can be used as a pairwise similarity measure. We also transformed Gower's distance  $d$  to  $\exp(-d)$  to become a similarity metric. The plot of the LC measure with respect to the order  $q$  for the two types of similarity metrics is given in **Supplemental Figure 1** for the three habitats.



**Supplemental Figure 1.** Diversity profiles as a function of the order  $q$  ( $0 \leq q \leq 5$ ) of the measure by Leinster & Cobbold (2012) for three habitats. (*Left panel*) The similarity is defined as one complement of Gower's distance: (*black line*) EM (in range: 2.09~2.01, when  $q$  is increased from 0 to 5), (*red line*) MO

(in range: 2.28~ 2.21), and (*blue line*) TR (in range: 2.31~ 2.24). (*Right panel*) The similarity is defined as  $\exp(-d)$  for Gower's distance  $d$ : (*black line*) EM (in range: 1.63~ 1.61), (*red line*) MO (in range: 1.71~ 1.69), and (*blue line*) TR (in range: 1.73~ 1.71). Abbreviations: EM, embryo dune; MO, mobile dune; TR, transition dune.

The two plots in **Supplemental Figure 1** reveal that the LC measure takes values in a very narrow range that hardly changes for the above two types of similarity matrices. Because the order  $q$  controls the measure's sensitivity to species relative abundances and a larger value of  $q$  places progressively more weight on common species, these plots demonstrate that the LC measure may not be sensitive to the species abundances. We have found similar patterns for many other data sets. Thus, a related question regards how the magnitude and “effective numbers” of the LC measure should be interpreted.

Recently, Reeve et al. (2014) proposed formulas for the alpha, beta, and gamma diversities based on the LC measure and on the decomposition framework of the ordinary Hill numbers. Here we consider the simplest equal-weight case and apply formulas by Reeve et al. (2014) to a simple similarity matrix. Consider two communities each with four species (1, 2, 3, 4). The relative abundances of the four species in Community I are 0.98, 0.003, 0.001, and 0.016. The relative abundances of the same four species for Community II are 0.90, 0.009, 0.082, and 0.009. Assume that the following matrix gives the pairwise similarity for the four species:

$$\begin{bmatrix} 1 & 0.9 & 0.9 & 0 \\ 0.9 & 1 & 0 & 0 \\ 0.9 & 0 & 1 & 0.9 \\ 0 & 0 & 0.9 & 1 \end{bmatrix}.$$

Then we obtain the following alpha and gamma diversities for four values of  $q$ :

Order	Gamma	Alpha
$q = 0$	1.2605	1.5375
$q = 0.5$	1.1120	1.1570
$q = 1$	1.0611	1.0679
$q = 2$	1.0343	1.0345

For this case, the gamma LC measure is less than the alpha LC measure not only for the four specific values of  $q$  in the above table, but also for all values of  $q \geq 0$ . This situation violates the necessary condition that alpha must always be less than or equal to gamma.

Leinster & Cobbold (2012, p. 478) indicated that their metric has close connections with the phylogenetic indexes of Faith (1992) and Chao et al. (2010). This may be a misleading statement. In their appendix, Leinster & Cobbold (2012) demonstrated that their formula could include Faith's *PD* and the phylogenetic Hill number of Chao and colleagues only for a particular constructed similarity matrix (possibly nonsymmetric) and species abundances. Note that their particular similarity matrix for species depends on the species relative abundance. Thus, when two communities have the same set of species with different sets of species abundances, the corresponding particular similarity matrices are different. Even within a single community, if two samples result in different species abundances, then LC's particular similarity matrices are different. Thus, the "connection" between their metric and Faith's *PD* and the measure of Chao and colleagues is based only on an uninterpretable similarity matrix. A useful "connection" between two measures should be based on a broad class of similarity matrices, not just on a single particular constructed matrix.

When a similarity matrix is not a naive identity matrix, the only general connection that we have found between the LC measure and the phylogenetic Hill numbers of Chao et al. (2010) occurs when the similarity matrix is obtained from an ultrametric tree and  $q = 2$ . That is, for any ultrametric tree, we can divide each species' pairwise phylogenetic distance by the tree depth so that all distances are scaled to be in the range  $[0, 1]$ . When the similarity between any two species is defined as the complement of the scaled distance, the LC measure for  $q = 2$  reduces to the phylogenetic Hill number of Chao and colleagues of the same order. However, nearly all similarity matrices calculated from species traits are nonultrametric. Therefore, this connection for  $q = 2$  is rarely valid in functional analysis.

## **2. SCHEINER APPROACH**

Scheiner (2012) also proposed a metric that integrates abundance, phylogeny, and function using a framework of Hill numbers. Our framework (attribute diversity and generalized Hill numbers) is also based on Hill numbers. However, the two approaches are completely different. In the following, we describe the fundamental concept of our unified approach and discuss the differences between our framework and Scheiner's approach.

### **2.1. The Basic Difference**

The major difference between our framework and Scheiner's approach lies in the interpretation of Hill numbers. In Scheiner's (2012) approach, the ordinary Hill numbers are interpreted as the variability in relative abundances among species. Using this approach, Scheiner's phylogenetic diversity quantifies the variability of proportional phylogenetic divergences of species, and his functional diversity quantifies the variability of proportional functional distinctiveness.

Our interpretation of Hill numbers is different. Our fundamental concept is based on the fact that there is a unique idealized assemblage with equally abundant species so that the actual assemblage and this idealized assemblage have the same diversity of order  $q$ . Thus, our extension to phylogenetic diversity and functional diversity leads to completely different measures from those of Scheiner as briefly described below.

**2.1.1. Phylogenetic diversity measures.** Our phylogenetic Hill number (or mean phylogenetic diversity) of order  $q$ , denoted by  ${}^q\overline{D}(\overline{T})$ , is the effective number of equally abundant and equally phylogenetically distinct species or lineages with a constant branch length  $\overline{T}$  from the root node. Here  $\overline{T}$  denotes the abundance-weighted mean distance from a tip node to the root node (for the definition of  $\overline{T}$ , see figure 1 of Chao et al. 2010). For an ultrametric tree with tree depth  $T$ ,  $\overline{T}$  reduces to the tree depth  $T$  and the measure is simply denoted by  ${}^q\overline{D}(T)$ . Generally, if  ${}^q\overline{D}(\overline{T}) = z$ , then the phylogenetic Hill number of the assemblage is the same as the diversity of an idealized assemblage consisting of  $z$  equally abundant and (phylogenetically) equally distinct lineages, all with branch length  $\overline{T}$  from the root node. In effect, there exists a unique idealized assemblage with equally abundant and equally distinct species or lineages so that the actual assemblage and this idealized assemblage have the same diversity of order  $q$ .

The phylogenetic Hill number (in units of “species equivalent”) does not incorporate information about the actual depth of the phylogenetic tree. To incorporate this depth, we also proposed the phylogenetic diversity  ${}^qPD(\overline{T})$  (in units of “lineage length”). For the ultrametric case with tree depth  $T$ , the measure  ${}^qPD(\overline{T})$  equals  $T \times {}^q\overline{D}(T)$  and is denoted by  ${}^qPD(T)$ . Thus, we have a measure in units of species equivalents as well as a measure in units of lineage length.

This is more useful biologically because the measure  ${}^qPD(\bar{T})$  quantifies the amount of evolutionary history in the tree (with branches weighted by the size of their contribution to the present-day assemblage) and is also fruitful mathematically because we then can link our measures to Faith  $PD$  (for  $q = 0$ ), phylogenetic entropy (for  $q = 1$ ), and Rao's quadratic entropy (for  $q = 2$ ). Scheiner's measure cannot be linked to the phylogenetic entropy or to Rao's quadratic entropy in general cases.

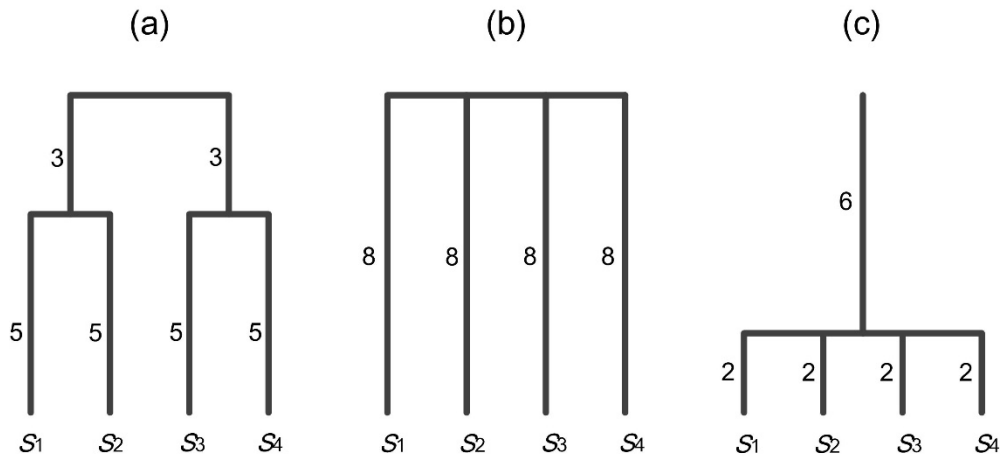
**2.1.2. Functional diversity measures.** Our functional Hill number denoted by  ${}^qD(Q)$  (see Table 1 of the main text) is interpreted as “the effective number of equally abundant and (functionally) equally distinct species.” Thus, if  ${}^qD(Q) = v$ , then the functional Hill number of order  $q$  of the actual assemblage is the same as that of an idealized assemblage having  $v$  equally abundant and equally distinct species with a constant distance  $Q$  for all species pairs. Our concept for functional diversity is based on the fact that there exists a unique idealized assemblage with equally abundant and equally distinct species so that the actual assemblage and this idealized assemblage have the same diversity of order  $q$ .

As with our phylogenetic Hill numbers, the functional Hill numbers  ${}^qD(Q)$  (in units of species equivalent) are scale free, so they need to be converted to our functional diversity  ${}^qFD(Q)$  (the effective total functional distance between species), defined as  ${}^qFD(Q) = Q \times [{}^qD(Q)]^2$ . Thus, we can link our measures to  $FAD$  (for  $q = 0$ ) and to the weighted Gini-Simpson index (for  $q = 2$ ) defined by Guiasu & Guiasu (2011, 2012) (see the main text for details). To our knowledge, Scheiner's metric cannot be linked to these two previous measures in general cases.

## 2.2. Different Meanings of Species Equivalents or Effective Number of Species

Scheiner's integrated metric and our phylogenetic (and functional) Hill number are both in units of species equivalents, which is interpreted as the equally abundant and equally distinct species. However, the definition of equally distinct diverges between Scheiner's approach and ours. We use a simple example to illustrate the two different meanings.

**2.2.1. Phylogenetic diversity measures.** Consider the following three assemblages with ultrametric cladograms. Each assemblage includes four species, and the tree depth is  $T = 8$ . The number along each branch denotes the length of that branch. For each assemblage, we assume that all four species are equally abundant.



For the above three cladograms for  $T = 8$ , **Supplemental Table 1** shows our phylogenetic Hill numbers  ${}^q\overline{D}(T)$  (in units of species equivalents), phylogenetic diversity  ${}^qPD(T)$  (in units of lineage length), and Scheiner's phylogenetic diversity.



**Supplemental Table 1.** Phylogenetic diversity measures for three assemblages

Measure	Order	Assemblage/cladogram		
		(a)	(b)	(c)
Chao et al. (2010)	$q = 0$	26	32	14
Phylogenetic	$q = 1$	24.78	32	11.31
diversity ${}^qPD(T)$	$q = 2$	23.27	32	9.85
Chao et al. (2010)	$q = 0$	3.25	4	1.75
Phylogenetic Hill	$q = 1$	3.08	4	1.41
number ${}^q\bar{D}(T)$	$q = 2$	2.91	4	1.23
Scheiner (2012)	$q = 0$	4	4	4
Phylogenetic	$q = 1$	4	4	4
diversity	$q = 2$	4	4	4

All the above three cladograms have the same proportional divergences as defined by Scheiner. For any  $q \geq 0$ , his phylogenetic diversity quantifies the variability of proportional phylogenetic divergences of species. Thus, it yields four equally distinct species for all three assemblages. When his measure takes a maximum value of 4, the assemblage may correspond to the four equally abundant species in cladograms *a*, *b*, and *c* or in any other symmetric or balanced cladograms. This explains why Scheiner (2012, p. 1195) indicated that his metric is a measure of tree symmetry or balance. His measure cannot distinguish the difference among the three assemblages; thus, species equivalents does not have a unique reference assemblage.

Our phylogenetic measures  ${}^q\bar{D}(\bar{T})$  and  ${}^qPD(\bar{T})$  both satisfy the “weak monotonicity”

property (Chao et al. 2010). This property requires that if a newly added rarest species is maximally distinct from all other species in the assemblage, then a phylogenetic measure should not decrease. However, Scheiner's phylogenetic diversity measure does not satisfy this property. For  $q > 0$ , if such a species is added to assemblage  $a$  or  $c$  shown above, then that tree becomes nonsymmetric, implying a possible decline in a measure of symmetry.

In Scheiner's measure, equally distinct means species are equally divergent from the age of the root node. Our definition of equally distinct (in the effective sense) implies that any two species must have a constant phylogenetic distance of  $\bar{T}$  (or  $T$  in ultrametric cases). For example, in cladogram  $a$ , the distance between species 1 and species 2 is 5, whereas the distance between 1 and species 3 is 8, so the four species in cladogram  $a$  are not equally distinct in our perspective. Similarly, the four species in cladogram  $c$  are not equally distinct with branch length of 8 as in the idealized assemblage. Only cladogram  $b$  is the unique idealized assemblage: All species are equally distinct with branch length of 8. Thus, for the effective number of species in our phylogenetic diversity measure, there exists a unique reference assemblage so that the actual assemblage and this idealized assemblage have the same diversity of order  $q$ . For example, in the special case of  $q = 0$ , the phylogenetic Hill number of cladogram  $c$  is 1.75. Then this means the zero-order diversity of the assemblage is the same as an idealized assemblage with 1.75 equally abundant species or lineages and all branch lengths are 8, i.e., the idealized reference assemblage is like cladogram  $b$  but with only 1.75 species. **Supplemental Table 1** reveals that, when diversity is based on our phylogenetic Hill number  ${}^q\bar{D}(T)$  and phylogenetic diversity  ${}^qPD(T)$ , the three assemblages for any  $q$  have consistent ordering:  $b > a > c$ , whereas Scheiner's measure shows  $a = b = c$ . Ecologists may use this example to choose which measure to employ in their analysis.

**2.2.2. Functional diversity measures.** We use a simple example to compare the difference between our functional diversity measures and Scheiner's approach. Consider the following example: In assemblage *a*, all *S* species are equally distinct with species pairwise distance  $d_{ij} = 0.1$  units. In assemblage *b*, all *S* species are equally distinct with  $d_{ij} = 0.9$  units. Scheiner's functional diversity quantifying the variability of functional distinctiveness will give the same functional diversity for these two assemblages. Yet, from our approach, there are *S* species with a constant distance of 0.1 for all species pairs in assemblage *a*, and our functional diversity (i.e., effective total distance) between species is  $S^2 \times 0.1$ . However, for assemblage *b*, there are *S* species with a constant distance of 0.9 for all species pairs, and the functional diversity is  $S^2 \times 0.9$ . The effective numbers of species are the same for the two assemblages, but the total distances between species for the two assemblages are different. Thus, Scheiner's measure loses the information about the magnitude of species pairwise distances, which we think is important to characterize distance-based traits diversity.

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