Chun-Huo Chiu, Lou Jost, and Anne Chao. 2013. Phylogenetic beta diversity, similarity, and differentiation measures based on Hill numbers. *Ecological Monographs*.

Appendix F: A simple hypothetical tree with completely distinct lineages

In Example 1 of the main text, we considered two assemblages of landlocked organisms (Fig. F1) that originated on a super-continent that broke into two parts. Assume that the two assemblages evolved in isolation for approximately T years. Although this example is simple, it provides an initial comparison so that the analyses for more complicated example and real data can be better understood.
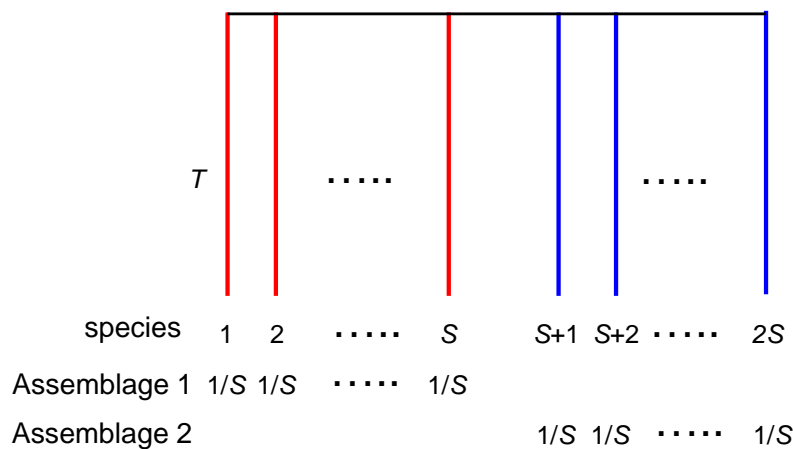

Fig. F1: A simple hypothetical tree. All S species in each assemblage diverged from their common ancestor T years ago, and all species are equally common in each assemblage.

(1) $q = 2$ case

Let us first apply Rao's quadratic entropy Q, the most frequently used measure that incorporates both abundances and phylogeny, to this simple tree (Fig. F1). Usually the distance measure used is the branch length in years connecting any two individuals in the assemblage to their most recent common node. Then Rao's quadratic entropy, in its non-normalized form, is the mean divergence time between two randomly chosen individuals of an assemblage. In this example, the divergence time between two individuals is zero if they belong to the same species, and T otherwise (see Fig. F1). If there are S species in each continental assemblage, the quadratic entropy Q of each continent will be $0 \times (1/S) + T \times (1-1/S) = T(1-1/S)$. This would be the alpha quadratic entropy Q_α of the assemblages. For any fixed T, the alpha value will be high (i.e., tends to the maximum possible value of T) if and only if species richness S is high. The gamma value is the quadratic entropy of the pooled assemblage, $Q_\gamma = T[1-1/(2S)]$. For traditional additive partitioning based on quadratic entropy, the quadratic entropy excess or "beta" diversity is defined as gamma minus alpha, in this case $Q_\gamma - Q_\alpha = T/(2S)$. When S is high, this "beta" diversity necessarily approaches zero, even though the lineages of the two assemblages are completely

distinct (no shared lineages) since the date of the root of the tree.

The "differentiation" measure $J_{2N}(T)$ is obtained by dividing this "beta" by the gamma quadratic entropy (e.g. Hardy and Senterre 2007). A value near zero would be interpreted as indicating little or no differentiation, while a value near unity would be interpreted as indicating high differentiation. However, in this case the differentiation measure reduces to $J_{2N}(T) = [T/(2S)]/[T - T/(2S)] = 1/(2S-1)$, a number that approaches zero when alpha is high (equivalently, when S is high), even though the two assemblages are completely distinct and have been evolving independently since time T. Our theoretical result in the main text implies that when the within-assemblage quadratic entropy is high, the additive "differentiation" measure based on quadratic entropy always tends to zero for any assemblages, not just for simple completely distinct trees. These behaviors of additive "beta" and differentiation "beta"/gamma are exactly like the well-known problems of its parent measure, the Gini-Simpson index (Jost 2006, 2007, Hardy and Jost 2008). Similar findings hold for more complicated trees and real data as shown in the main text. In Fig. F2 (left panel), we show the pattern of the differentiation $J_{2N}(T)$ as a function of species richness. This function is decreasing to 0 as S is large. The measure $J_{2N}(T)$ is independent of T, as shown in Fig. F2 (right panel) specifically for $S = 10$.

Biologists using Q to make conservation decisions for this imaginary set of continents with large S will conclude that since the additive "differentiation" measure is near zero, the second continent is superfluous and need not be a conservation priority. Yet the assemblages are equally diverse and share no species, and have been evolving in isolation since time T, so each may consist entirely of endemic genera or families.

Now turn to our proposed phylogenetic beta diversity (Eq. 10b in the main text) for $q = 2$, with our temporal perspective T as the age of the continental split (the age of the basal node).
$$^2\overline{D}_\beta(T) = (1 - Q_\gamma/T)^{-1}/(1 - Q_\alpha/T)^{-1} = (T/S)^{-1}/(T/2S)^{-1} = 2,$$
implying that there are two distinct assemblages, as expected. All the differentiation measures (see Table 1 of the main text) take the maximum possible value of unity for all S. For examples, the proposed differentiation measures $1 - \overline{C}_{2N}(T)$ and $1 - \overline{U}_{2N}(T)$ are

$$1 - \overline{C}_{2N}(T) = \frac{1 - [1/^2\overline{D}_\beta(T)]}{1 - 1/N} = 1,$$

$$1 - \overline{U}_{2N}(T) = \frac{^2\overline{D}_\beta(T) - 1}{N - 1} = 1.$$

This is consistent with our intuition, because the two assemblages are completely distinct after time T, so the differentiation should attain the maximum value of unity.

(2) $q = 1$ case

For $q = 1$, traditional additive decomposition is based on the phylogenetic entropy $H_P = -\sum_i L_i a_i \log a_i$. For the tree in Fig. F1, we have the alpha value $H_{P,\alpha} = T(\log S)$, and the gamma value $H_{P,\gamma} = T[\log(2S)]$. The additive "beta" (phylogenetic entropy excess) is $H_{P,\gamma} - H_{P,\alpha} = T(\log 2)$, and the "differentiation" measure $J_{1N}(T) = (\log 2)/[\log(2S)]$. When gamma is high

(equivalently, when S is large), this differentiation measure tends to zero (Fig. F2, left panel), supposedly indicating no differentiation, even though the two assemblages are completely distinct. This counter-intuitive behavior will arise for all trees, not just for simple completely distinct trees. As we have proved in Theorem E1 of Appendix E, traditional additive "beta" entropy for any tree is bounded by $T \log N$, implying "beta"/gamma always tends to zero if gamma is large. Although in the case of $q = 1$, alpha and "beta" (H_P excess) are independent, "beta"/gamma is not a legitimate measure of differentiation (because the numerator and denominator do not obey the Replication Principle). As shown in Table 1 of the main text, dividing "beta" by $T \log N$, we obtain the correct differentiation value of unity for this example.

When assemblage weights are equal, our proposed beta in terms of phylogenetic entropy is given in Eq. 10a for $q = 1$. For any temporal perspective T, we have

$$^{1}\overline{D}_{\beta}(T) = \exp[(H_{P,\gamma} - H_{P,\alpha})/T] = \exp(\log 2) = 2,$$

indicating that there are two completely distinct assemblages. The proposed differentiation measures are $1 - \overline{U}_{1N}(T) = 1 - \overline{C}_{1N}(T) = \log {}^{1}\overline{D}_{\beta}(T)/\log N = \log 2/\log 2 = 1$ (see Table 1 of the main text for $N = 2$) for all S and all T; see Fig. F2.

(3) $q = 0$ case

The phylogenetic generalized entropy for the case $q = 0$ is based on $^{0}I(T) =$ total branch length $L(T)$ minus tree height T. For the simple tree in Fig. F1, we have gamma branch length $L_{\gamma}(T) = 2TS$ and alpha branch length $L_{\alpha}(T) = TS$. Thus, the alpha value $^{0}I_{\alpha}(T) = L_{\alpha}(T) - T = (S-1)T$ and the gamma value $^{0}I_{\gamma}(T) = L_{\gamma}(T) - T = (2S-1)T$, implying the additive "beta" is ST. Clearly, this beta is positively constrained by alpha for any fixed T. The "differentiation" in this special case is $J_{0N}(T) = S/(2S-1)$. When S is large enough, this differentiation measure tends to the value of $1/2$ (see Fig. F2) for this example and in general it tends to $1-1/N$ for N completely distinct assemblages. For small values of S, this differentiation measure gives a value that is different from $1/2$ (Fig. F2).

Our proposed beta for $q = 0$, for any temporal perspective T, is $^{0}\overline{D}_{\beta}(T) = L_{\gamma}(T)/L_{\alpha}(T) = 2$, correctly indicating two completely distinct assemblages in the region. Our proposed differentiation measure is given in Table 1 in terms of tree length turns out again to correctly take its maximum possible value of unity. That is,

$$1 - \overline{C}_{0N}(T) = \frac{L_{\gamma}(T)/L_{\alpha}(T) - 1}{N - 1} = 1;$$

$$1 - \overline{U}_{0N}(T) = \frac{1 - L_{\alpha}(T)/L_{\gamma}(T)}{1 - 1/N} = 1.$$

The upper bound in Eq. 13b of the main text for the traditional additive "beta" in this case reduces to $(N-1)[T + {}^{0}I_{\alpha}(T)] = ST$. Dividing the additive "beta" $^{0}I_{\gamma}(T) - {}^{0}I_{\alpha}(T) = ST$ by this upper bound, we see the normalized value is equal to unity for all S and all T; see Fig. F2. Similarly, the upper

bound in Eq. 13d for the traditional additive "beta" reduces to $(N^{-1}-1)[T + {}^{0}I_{\gamma}(T)] = ST$. Again, the normalized value is equal to unity for all S and all T.

In summary, for the simplest tree for a pair of assemblages with completely distinct lineages, defined in Fig. F1, our proposed normalized phylogenetic differentiation measures $1-\overline{C}_{qN}(T)$ and $1-\overline{U}_{qN}(T)$ (based on our mean phylogenetic diversity) are always 1 for all $q = 0, 1, 2$, and all richnesses S and all temporal perspective T, indicating that we have two completely distinct assemblages over this time interval; see Fig. F2. In contrast, the traditional differentiation measure $J_{qN}(T)$ (based on phylogenetic generalized entropies) depends on S. We have $J_{2N}(T) = 1/(2S-1)$, $J_{1N}(T) = (\log 2)/[\log(2S)]$, and $J_{0N}(T) = S/(2S-1)$. As shown in Fig. F2 (right panel) for $S = 10$, $J_{2N} = 0.053$, $J_{1N} = 0.23$ and $J_{0N} = 0.53$. The left panel of Fig. F2 shows, as S tends to be large, that both J_{2N} and J_{1N} approach to zero and J_{0N} approaches $1/2$. These erratic behaviors show that traditional approach based on phylogenetic generalized entropies does not work even for the simplest trees. However, as we have proved in Theorems E1 and E2 in Appendix E, traditional approach can be easily fixed by normalization. The normalized measures turn out to be the proposed differentiation measures $1-\overline{C}_{qN}$ and $1-\overline{U}_{qN}(T)$.
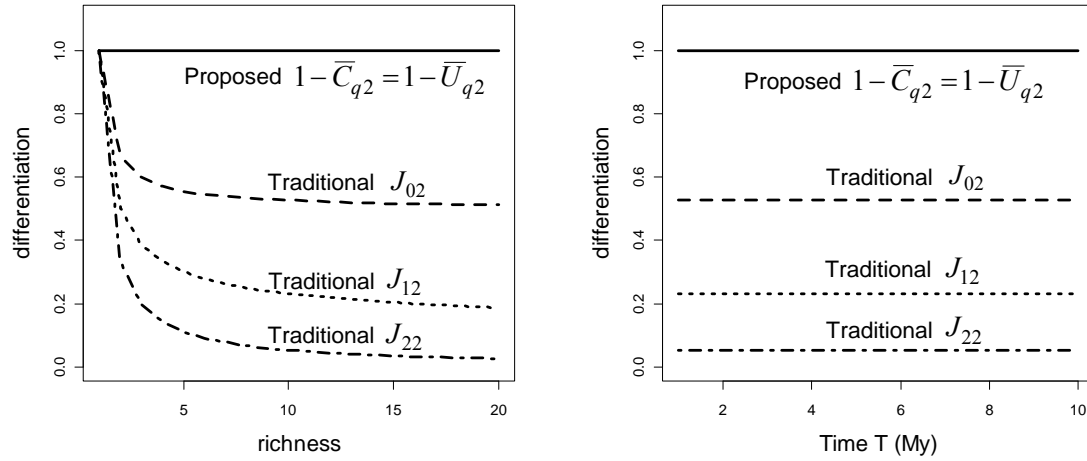

Fig. F2: Comparison of the proposed differentiation measures, $1-\overline{C}_{qN}(T)$ and $1-\overline{U}_{qN}(T)$ (based on our mean phylogenetic diversity) and the traditional differentiation measure $J_{qN}(T)$ (based on the traditional additive partitioning of phylogenetic generalized entropy).
(Left panel) Plots of the differentiation measures as a function of species richness. All measures are independent of the value of T. Both the proposed measures, $1-\overline{C}_{qN}(T)$ and $1-\overline{U}_{qN}(T)$, are unity for all $q = 0, 1, 2$ and all richness S. The measure $J_{qN}(T)$ depends on q: for $q = 0$, measure tends to 1/2 when S is large; for $q = 1$, measure tends to 0 when S is large; for $q = 2$, measure tends to 0 when S is large.
(Right panel) Plots of the differentiation measures as a function of T given $S = 10$ for $q = 0, 1$ and 2.

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