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APPENDIX E. Mathematical flaws in the traditional additive approach based on generalized entropy excess or phylogenetic generalized entropy excess

Non-phylogenetic approach based on the generalized entropies

When our goal is to measure similarity and differentiation among multiple assemblages, traditional approach that incorporates species relative abundances has been based on additive partitioning of generalized entropy qH (including Shannon entropy and the Gini-Simpson index) or phylogenetic generalized entropy ${}^qI(T)$ (including phylogenetic entropy H_P and quadratic entropy Q). We first review the non-phylogenetic version (Jost 2006, 2007 and Jost et al. 2010) so that readers can better understand what the mathematical flaws are in the additive approach. Since the generalized entropies ${}^qH = (1 - \sum_i p_i^q)/(q-1)$ include Shannon entropy and the Gini-Simpson index as special cases, our discussion is focused on the additive “beta” based on the generalized entropy excess. Since the “beta” diversity for the Gini-Simpson index is related to our measure only in the equal-weight case (see Table 1 of the main text), we focus on the equal-weight case and show how to fix and connect the additive measures to our measures.

Let ${}^qH_\gamma$ and ${}^qH_\alpha$ denote respectively the gamma and alpha generalized entropies. The additive “beta” (generalized entropy excess) is defined as ${}^qH_\beta = {}^qH_\gamma - {}^qH_\alpha$. Jost et al. (2010, p. 73, their Eq. 8) proved the following relationships which show how the additive “beta” is constrained by alpha generalized entropy (equivalently by gamma generalized entropy, as will be shown later of this Appendix):

$$0 \leq {}^qH_\beta = {}^qH_\gamma - {}^qH_\alpha \leq \frac{(1 - N^{1-q})[1 - (q-1)({}^qH_\alpha)]}{q-1}, \quad q \neq 1. \quad (\text{E.1})$$

$$0 \leq {}^1H_\beta = {}^1H_\gamma - {}^1H_\alpha \leq \lim_{q \rightarrow 1} \frac{(1 - N^{1-q})[1 - (q-1)({}^qH_\alpha)]}{q-1} = \log N. \quad (\text{E.2})$$

We discuss the following three special cases in detail so that we can transparently see how the generalized entropy excess depends on alpha for each order $q = 0, 1$ and 2 .

(1) $q = 2$ case

For $q = 2$, Eq. (E.1) gives the inequality $H_{GS,\gamma} - H_{GS,\alpha} \leq (1 - 1/N)(1 - H_{GS,\alpha})$, where $H_{GS,\gamma}$ and $H_{GS,\alpha}$ denote respectively gamma and alpha Gini-Simpson measures. This shows that the “beta” Gini-Simpson is confounded with alpha, and is negatively constrained by alpha. When the alpha Gini-Simpson is high (i.e., when $H_{GS,\alpha}$ tends to 1), the maximum value of “beta”, $(1 - 1/N)(1 - H_{GS,\alpha})$, tends to 0. So the “beta” Gini-Simpson is necessarily to be small, regardless of the actual differentiation between groups. In this case, the differentiation measure

“beta”/gamma always approaches zero, and the similarity measure alpha/gamma always approaches unity (Jost 2006, 2007), supposedly indicating a high degree of similarity between groups, even when the groups are completely dissimilar (no shared species). Due to this dependence on alpha, the additive “beta”/gamma based on the Gini-Simpson index does not measure differentiation, and alpha/gamma does not measure compositional similarity. One way to fix this (Jost et al. 2010) is to normalize the additive “beta” by dividing it by its upper limit given the observed values of alpha and N , yielding $(H_{GS,\gamma} - H_{GS,\alpha}) / [(1 - 1/N)(1 - H_{GS,\alpha})]$, which is identical to our equal-weight differentiation measure $1 - C_{2N}$ (see Table 1 of the main text).

(2) $q = 1$ case

For $q = 1$, Eq. (E.2) shows that the additive “beta” entropy is bounded by a constant $\log N$, not on alpha, as the additive partitioning for entropy really is a complete partitioning. So under an additive framework, traditional differentiation as measured by (“beta” entropy)/(gamma entropy) must tend to zero if the denominator (gamma entropy) is large. This partly explains why, even though additive “beta” entropy measures pure differentiation, additive “beta”/gamma based on entropy is not a proper differentiation measure. (Another reason is that entropies do not obey the Replication Principle). Also, when gamma Shannon entropy is high, the so-called similarity measure alpha/gamma approaches unity. Thus the additive alpha/gamma based on entropy does not measure compositional similarity (again, because entropies do not obey the Replication Principle). It is also readily seen from Eq. (E.2) that for entropy, instead of using beta/gamma, one should use the normalized measure “beta”/($\log N$) in the range $[0, 1]$ as a proper differentiation measure. As shown in Chao et al. (2012), entropy “beta”/($\log N$) is identical to equal-weight $1 - C_{1N}$ measure defined in Table 1 of the main text.

Thus, the additive approach applied to the two concave measures (entropy and Gini-Simpson index, which is a generalized entropy) may lead to inconsistent conclusions and biologically misleading interpretations (Jost 2006, 2007). All authors in a recent Forum on diversity partitioning (Ellison 2010 and papers following it) therefore agreed that diversity measures should be based on Hill numbers instead of Shannon entropy and the Gini-Simpson measure.

(3) $q = 0$ case

For $q = 0$, Eq. (E.1) is equivalent to the constraint $S - \bar{S} \leq (N - 1)\bar{S}$, where S denotes species richness in the pooled assemblage (gamma species richness) and \bar{S} denotes the average species richness in an individual assemblage (alpha species richness). Eq. (E.1) implies that the “beta” species richness is confounded with alpha, and is positively constrained by alpha. The generalized entropy of order 0 is species richness minus one, but here we just use species richness instead because the latter is the measure that has been considered for diversity decomposition. Based on species richness, the differentiation measure “beta”/gamma $= (S - \bar{S}) / S = (1 - 1/N)(1 - U_{0N})$ where U_{0N} is the homogeneity measure defined in Table 1 of the main text. Thus, “beta”/gamma based on species richness can be used as a differentiation measure, but its range still depends on N since it ranges from 0 (when all assemblages are identical) to $1 - 1/N$ (when all assemblages have no shared species). Our approach is to remove the dependence of the additive “beta” on alpha by using a normalized measure $(S - \bar{S}) / [(N - 1)\bar{S}]$, which is identical to $1 - C_{0N}$ (see Table 1 of the main text). The normalized measure is always in the range $[0, 1]$ so it can be compared across regions with different number of assemblages.

For a general order $q > 1$, Eq. (E.1) shows that additive “beta” generalized entropy is strongly *negatively* constrained by the value of alpha. If alpha generalized entropy of order $q > 1$ tends to the maximum possible value $1/(q-1)$, then the “beta” is necessarily to be small. In contrast, for $q < 1$, Eq. (E.1) shows that the additive “beta” generalized entropy is *positively* constrained by the value of alpha. As shown for the orders $q = 0$ and 2 above, the dependence of the additive generalized entropy “beta” on its alpha can be removed by dividing the additive “beta” by its maximum possible value in Eqs. (E.1) and (E.2). Based on those maximum values and the relationship between Hill numbers and generalized entropy, $(^qD)^{1-q} = 1 - (q-1)(^qH)$, we can readily show that the normalized measure turns out to be $1 - C_{qN}$. That is, for $q \neq 1$, we have

$$\begin{aligned} \frac{^qH_\gamma - ^qH_\alpha}{\max(^qH_\gamma - ^qH_\alpha)} &= \frac{(q-1)(^qH_\gamma - ^qH_\alpha)}{(1 - N^{1-q})[1 - (q-1)(^qH_\alpha)]} \\ &= \frac{1 - (q-1)(^qH_\alpha) - [1 - (q-1)(^qH_\gamma)]}{(1 - N^{1-q})[1 - (q-1)(^qH_\alpha)]} \\ &= \frac{1 - (^qD_\beta)^{1-q}}{1 - N^{1-q}} = 1 - C_{qN}. \end{aligned} \quad (\text{E.3})$$

For $q = 1$, the entropy “beta” should be normalized by the upper bound $\log N$. The normalized measure becomes

$$\frac{^1H_\gamma - ^1H_\alpha}{\max(^1H_\gamma - ^1H_\alpha)} = \frac{(^1H_\gamma - ^1H_\alpha)}{\log N} = 1 - C_{1N}. \quad (\text{E.4})$$

The dependence relationship in Eq. (E.1) is equivalent to the following constraint which shows how the additive “beta” generalized entropy depends on gamma generalized entropy:

$$0 \leq ^qH_\beta = ^qH_\gamma - ^qH_\alpha \leq \frac{(1/N^{1-q} - 1)[1 - (q-1)(^qH_\gamma)]}{q-1}, \quad q \neq 1; \quad (\text{E.5})$$

$$0 \leq ^1H_\beta = ^1H_\gamma - ^1H_\alpha \leq \lim_{q \rightarrow 1} \frac{(1/N^{1-q} - 1)[1 - (q-1)(^qH_\gamma)]}{q-1} = \log N. \quad (\text{E.6})$$

Parallel discussion to those for the dependence on alpha can be made. Here we only single out the special case of $q = 2$. In this case, Eq. (E.5) gives the constraint $H_{GS,\gamma} - H_{GS,\alpha} \leq (N-1)(1 - H_{GS,\gamma})$. This shows that the “beta” Gini-Simpson is also negatively confounded with gamma. When the gamma Gini-Simpson is high (i.e., $H_{GS,\gamma}$ tends to 1), the maximum value of “beta”, $(N-1)(1 - H_{GS,\alpha})$, tends to 0. So the “beta” Gini-Simpson is necessarily to be small. We note that for the Gini-Simpson index, Eq. (C.7) in Appendix C implies that $(1 - H_{GS,\gamma})^{-1} \leq N(1 - H_{GS,\alpha})^{-1}$. Thus, for a fixed N , $H_{GS,\gamma}$ tends to 1 if and only if $H_{GS,\alpha}$ tends to 1. The condition “alpha Gini-Simpson is high” is equivalent to the condition “gamma Gini-Simpson is high”.

For a general order of q , we can remove the gamma-dependence by normalization. Dividing

${}^qH_\gamma - {}^qH_\alpha$ by its maximum, the normalized measure turns out to be $1 - U_{qN}$. That is,

$$\frac{(q-1)({}^qH_\gamma - {}^qH_\alpha)}{(1/N^{1-q} - 1)[1 - (q-1)({}^qH_\gamma)]} = \frac{[1/{}^qD_\beta]^{1-q} - 1}{1/N^{1-q} - 1} = 1 - U_{qN}. \quad (\text{E.7})$$

For $q = 1$, the entropy “beta” should be normalized by the upper bound $\log N$ in Eq. (E.6). The normalized measure becomes

$$\frac{{}^1H_\gamma - {}^1H_\alpha}{\max({}^1H_\gamma - {}^1H_\alpha)} = \frac{({}^1H_\gamma - {}^1H_\alpha)}{\log N} = 1 - U_{1N} = 1 - C_{1N}. \quad (\text{E.8})$$

Thus eliminating the gamma dependence, we get a class of complementarity measures.

The above discussion shows the generality of the two classes of overlap measures C_{qN} and U_{qN} , because they are the normalized similarity measures that are common to both the additive approach based on generalized entropy and the approach based on Hill numbers.

Traditional additive framework based on the phylogenetic generalized entropies

We now extend the dependence relationships in Eqs. (E.1) and (E.2) to the phylogenetic generalizations in the following Theorem E1, and extend the dependence relationships in Eqs. (E.5) and (E.6) to the phylogenetic generalizations in the following Theorem E2.

Theorem E1: The phylogenetic generalized entropy excess (or the phylogenetic additive “beta” in the main text), ${}^qI_\beta(T) = {}^qI_\gamma(T) - {}^qI_\alpha(T)$, depends on alpha generalized entropy through the following inequality (see Eq. 13b, 13c in the main text)

$$0 \leq {}^qI_\beta(T) = {}^qI_\gamma(T) - {}^qI_\alpha(T) \leq \frac{(1 - N^{1-q})\{T - (q-1)[{}^qI_\alpha(T)]\}}{q-1}, \quad q \neq 1. \quad (\text{E.9})$$

For $q = 1$, we have

$$0 \leq {}^1I_\beta(T) = {}^1I_\gamma(T) - {}^1I_\alpha(T) \leq \lim_{q \rightarrow 1} \frac{(1 - N^{1-q})\{T - (q-1)[{}^qI_\alpha(T)]\}}{q-1} = T \log N. \quad (\text{E.10})$$

The normalized measures turn out to be:

$$\frac{[{}^qI_\gamma(T) - {}^qI_\alpha(T)]}{\max[{}^qI_\gamma(T) - {}^qI_\alpha(T)]} = \frac{(q-1)[{}^qI_\gamma(T) - {}^qI_\alpha(T)]}{(1 - N^{1-q})\{T - (q-1)[{}^qI_\alpha(T)]\}} = 1 - \bar{C}_{qN}(T), \quad q \neq 1; \quad (\text{E.11})$$

$$\frac{[{}^1I_\gamma(T) - {}^1I_\alpha(T)]}{\max[{}^1I_\gamma(T) - {}^1I_\alpha(T)]} = \frac{[{}^1I_\gamma(T) - {}^1I_\alpha(T)]}{T \log N} = 1 - \bar{C}_{1N}(T). \quad (\text{E.12})$$

Proof: From Eq. 2c of the main text, the phylogenetic generalized entropy can be expressed as

$${}^qI(T) = (T - \sum_{i \in B_T} L_i a_i^q) / (q-1).$$

Then we can obtain the relationship between ${}^qI(T)$ and our mean phylogenetic diversity $\bar{D}(T)$:

$${}^q\bar{D}(T) = \left\{ 1 - \frac{(q-1)[{}^qI(T)]}{T} \right\}^{1/(1-q)}. \quad (\text{E.13})$$

In Eq. (C.7) of Appendix C, we have proved ${}^q\bar{D}_\gamma(T) \leq N[{}^q\bar{D}_\alpha(T)]$, which is equivalent to

$$\left\{ 1 - \frac{(q-1)[{}^qI_\gamma(T)]}{T} \right\}^{1/(1-q)} \leq N \left\{ 1 - \frac{(q-1)[{}^qI_\alpha(T)]}{T} \right\}^{1/(1-q)}.$$

If $q < 1$, the above implies

$$\left\{ 1 - \frac{(q-1)[{}^qI_\gamma(T)]}{T} \right\} \leq N^{1-q} \left\{ 1 - \frac{(q-1)[{}^qI_\alpha(T)]}{T} \right\},$$

which then implies

$${}^qI_\gamma(T) - {}^qI_\alpha(T) \leq \frac{(1 - N^{1-q})\{T - (q-1)[{}^qI_\alpha(T)]\}}{q-1}.$$

For $q > 1$, we obtain exactly the same inequality. We thus finish the proof of (E.9). For the case of $q = 1$, Eq. (E.10) follows by direct computation. To obtain the normalized measure in Eq. (E.11), we note from Eq. (E.13),

$${}^q\bar{D}_\beta(T) = \frac{{}^q\bar{D}_\gamma(T)}{{}^q\bar{D}_\alpha(T)} = \frac{\{T - (q-1)[{}^qI_\gamma(T)]\}^{1/(1-q)}}{\{T - (q-1)[{}^qI_\alpha(T)]\}^{1/(1-q)}}.$$

This leads to the following for $q \neq 1$

$$\begin{aligned} \frac{[{}^qI_\gamma(T) - {}^qI_\alpha(T)]}{\max[{}^qI_\gamma(T) - {}^qI_\alpha(T)]} &= \frac{(q-1)[{}^qI_\gamma(T) - {}^qI_\alpha(T)]}{(1 - N^{1-q})\{T - (q-1)[{}^qI_\alpha(T)]\}} \\ &= \frac{T - (q-1)[{}^qI_\alpha(T)] - \{T - (q-1)[{}^qI_\gamma(T)]\}}{(1 - N^{1-q})\{T - (q-1)[{}^qI_\alpha(T)]\}} \\ &= \frac{1 - [{}^q\bar{D}_\beta(T)]^{1-q}}{1 - N^{1-q}} = 1 - \bar{C}_{qN}(T). \end{aligned}$$

The proof for the case of $q = 1$ is straightforward and thus omitted.

Theorem E2: The phylogenetic generalized entropy excess (or the phylogenetic additive “beta” in the main text), ${}^qI_\beta(T) = {}^qI_\gamma(T) - {}^qI_\alpha(T)$, depends on gamma generalized entropy through the following inequality (Eq. 13d in the main text)

$$0 \leq {}^q I_\beta(T) = {}^q I_\gamma(T) - {}^q I_\alpha(T) \leq \frac{(1/N^{1-q} - 1)\{T - (q-1)[{}^q I_\gamma(T)]\}}{q-1}, \quad q \neq 1. \quad (\text{E.14})$$

For $q = 1$, we have

$$0 \leq {}^1 I_\beta(T) = {}^1 I_\gamma(T) - {}^1 I_\alpha(T) \leq \lim_{q \rightarrow 1} \frac{(1/N^{1-q} - 1)\{T - (q-1)[{}^q I_\gamma(T)]\}}{q-1} = T \log N.$$

The normalized measures turn out to be:

$$\frac{[{}^q I_\gamma(T) - {}^q I_\alpha(T)]}{\max[{}^q I_\gamma(T) - {}^q I_\alpha(T)]} = \frac{(q-1)[{}^q I_\gamma(T) - {}^q I_\alpha(T)]}{(1/N^{1-q} - 1)\{T - (q-1)[{}^q I_\gamma(T)]\}} = 1 - \bar{U}_{qN}(T), \quad q \neq 1;$$

$$\frac{[{}^1 I_\gamma(T) - {}^1 I_\alpha(T)]}{\max[{}^1 I_\gamma(T) - {}^1 I_\alpha(T)]} = \frac{[{}^1 I_\gamma(T) - {}^1 I_\alpha(T)]}{T \log N} = 1 - \bar{C}_{1N}(T) = 1 - \bar{U}_{1N}(T).$$

Proof: In Eq. (C.8) of Appendix C, we have proved ${}^q \bar{D}_\gamma(T)/N \leq {}^q \bar{D}_\alpha(T)$. Then from Eq. (E.13), we have

$$\frac{1}{N} \left\{ 1 - \frac{(q-1)[{}^q I_\gamma(T)]}{T} \right\}^{1/(1-q)} \leq \left\{ 1 - \frac{(q-1)[{}^q I_\alpha(T)]}{T} \right\}^{1/(1-q)}.$$

The proof steps are then parallel to those in Theorem E1 and thus are omitted.

Generalizing to non-ultrametric cases

In Pavoine et al.'s (2009) original formulation (see Eq. 2d of the main text and Appendix A), phylogenetic generalized entropy can be defined only for ultrametric trees. We give a new formulation in Eq. 2c of the main text. We can readily extend Eq. 2c to non-ultrametric trees. That is, phylogenetic generalized entropy which is a function of mean base change \bar{T} can be formulated as

$${}^q I(\bar{T}) = [\bar{T} - \sum_{i \in B_{\bar{T}}} L_i a_i^q] / (q-1).$$

For the non-ultrametric cases we can extend Eq. (E.13) to the following relationship between our mean phylogenetic diversity and phylogenetic generalized entropy:

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

Then all conclusions in Theorems E1 and E2 can be similarly extended to the non-ultrametric cases by substituting \bar{T} for T . Therefore, all mathematical flaws associated with the ultrametric cases are also carried over to the non-ultrametric cases. However, normalization can be applied to fix the flaws and we obtain the same classes of similarity and differentiation measures as those in Table 1 of the main text.

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