1 **A multifaceted approach to analyzing taxonomic, functional and phylogenetic β -** 2 **diversity**

3 **Running title: A multifaceted approach to β -diversity**

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13 **Authors' declaration**

14 GN and LD conceived the idea, performed the analysis and wrote manuscript. WV and
15 YRS collected the data for stream fish communities and species traits, and constructed
16 the phylogenetic hypothesis used in this study.

17

18

19 **Abstract**

20 Ecological literature offers a myriad of methods for quantifying β -diversity. One such
21 methods is determining BD_{total} (BD), which, unlike other methods, can be decomposed
22 into meaningful components that indicate how unique a community is regarding its
23 composition (local contribution) and how unique a species is regarding its occurrence in
24 the metacommunity (species contribution). Despite this advantage, the original
25 formulation of the BD metric only assesses taxonomic variation and neglects other
26 important dimensions of biodiversity. We expanded the original formulation of BD to
27 capture variation in the functional and phylogenetic dimensions of a metacommunity by
28 computing two new metrics — BD_{Fun} and BD_{Phy} — as well as their respective
29 components that represent the local and species contribution. We tested the statistical
30 performance of these new metrics for capturing variation in functional and phylogenetic
31 composition through simulated metacommunities and illustrated the potential use of
32 these new metrics by analyzing β -diversity of stream fish communities. Our results
33 demonstrated that BD_{Phy} and BD_{Fun} have acceptable type I error and great power to
34 detect the effect of deep evolutionary relationships and attributes mediating patterns of
35 β -diversity. The empirical example illustrates how BD_{Phy} and BD_{Fun} reveal
36 complementary aspects of β -diversity relative to the original BD metric. These new
37 metrics can be used to identify local communities that are of conservation importance
38 because they represent unique functional, phylogenetic and taxonomic compositions.
39 We conclude that BD_{Phy} and BD_{Fun} are important tools for providing complementary
40 information in the investigation of the structure of metacommunities.

41 *Key-words:* functional beta diversity, phylogenetic β -diversity, fuzzy sets, local
42 contribution to beta diversity, statistical performance.

43 **Introduction**

44 Since Whitaker's seminal paper (Whittaker 1960), many measures and definitions have
 45 been proposed to refer to and operationalize β -diversity. Despite the diversity of
 46 mathematical formulations and propositions to operationalize this concept (Anderson et
 47 al. 2011 for a review), at the core of any β -diversity metric is the notion that it has the
 48 purpose of capturing patterns of variation in community composition (Legendre et al.
 49 2005), which in turn can be used to describe ecological patterns that can shed light on
 50 the processes and mechanisms that affect the distribution of species in space and time
 51 (Baselga 2010).

52 Among the plethora of methods to measure β -diversity is the framework called
 53 BD_{total} (hereafter only BD) proposed by Legendre & De Cáceres (2013), which deserves
 54 special attention due to its computational simplicity and the meaningful components
 55 that can be extracted from it. Among the advantages of this method we stress its
 56 mathematical independence (the ability to compute β -diversity independently of
 57 computing alpha and gama diversity) (Ellisson 2010), as well as the possibility to
 58 decompose the total variation present in a metacommunity matrix it into two
 59 components: Local Contribution to Beta Diversity (LCBD), which indicates the portion
 60 of total variation accounted for by an individual sample/community in a
 61 metacommunity, and Species Contribution to Beta Diversity (SCBD), which indicates
 62 the contribution of individual species to total BD. Whereas BD can be interpreted as a
 63 general measure of β -diversity for a metacommunity, LCBD and SCBD represent,
 64 respectively, how unique communities and species are in that metacommunity
 65 (Legendre and De Cáceres, 2013).

66 Despite the advantages of the BD framework and its components for revealing
67 ecological patterns in community structure (e.g. Li et al. 2019; Yao et al. 2019), it does
68 not consider variation from other dimensions of biodiversity that could shed light on
69 evolutionary and ecological patterns of species distributions across communities. It is
70 known that traditional taxonomic metrics of β -diversity combined with functional and
71 phylogenetic measures can shed light on the balance between environmental and
72 evolutionary factors affecting the composition of communities (Graham and Fine 2008;
73 Pillar et al. 2009; Pillar and Duarte 2010; Duarte et al. 2016; Safi et al., 2011). Among
74 the practical advantages of considering variation in different dimensions of biodiversity
75 is the possibility of identifying sites that concentrate functional, phylogenetic and
76 taxonomic diversity as being of special interest for conservation proposes (Devictor et
77 al. 2010). Consequently, statistical tools capable of characterizing variation in different
78 components of biological diversity are needed for improving our understanding of
79 factors acting on the structure of metacommunities.

80 Therefore, in order to join the advantages of the BD framework with the
81 possibility of capturing other components of variation in biological diversity, we show
82 herein how BD can be extended to produce β -diversity metrics that represent
83 phylogenetic and functional dimensions of diversity, while preserving all the advantages
84 of the original BD framework. Specifically, our goals were to: (1) expand the BD
85 framework by deriving two new metrics called BD_{Phy} and BD_{Fun} and their respective
86 components of local and species contributions to β -diversity; (2) test the performance of
87 BD_{Phy} , BD_{Fun} and their local components in capturing variation in metacommunity
88 composition and community uniqueness mediated by the functional and phylogenetic
89 relationship among species; and (3) show how these metrics can be used together to

90 reveal patterns of variation in metacommunities by using as an example a data base for
91 a tropical stream fish metacommunity.

92 **Methods**

93 *Expanding the BD framework to include functional and phylogenetic dimensions of*
94 *biodiversity.*

95 There are two ways to compute BD: directly from a matrix of species composition per
96 site, or from a distance matrix calculated from a species composition matrix using an
97 adequate dissimilarity index. For the sake of simplicity, we will demonstrate how BD
98 can be extended using only the procedure involving distance matrices.

99 Given a matrix **W** describing *i* sites (rows) by *j* species (columns), the first step
100 consists of redescribing the species occurrence matrix **W** to represent the clade and trait
101 distribution of species across communities (Pillar & Duarte, 2010; Duarte et al., 2016).
102 The redescription of matrix **W** to obtain the two new matrices starts by computing
103 phylogenetic and trait resemblance matrices, **S_p** and **S_f**, based on, phylogenetic tree and
104 species traits, respectively, as shown in Figure 1. The matrices **S_p** and **S_f** are
105 standardized by their column totals and multiplied by the transposition of matrix **W**
106 (steps 2.1 and 3.1 in Figure 1) to obtain matrix **P** that represents phylogenetic
107 composition and matrix **X** that represents the functional composition of communities.
108 Computing the square root of Bray-Curtis distance for **P** and **X** we obtain, respectively,
109 **D_p** and **D_f** (steps 2.2 and 3.2 in Figure 1), which describes pairwise distances (*D_{hi}*)
110 among communities (*n*) regarding clade and functional composition. These two distance
111 matrices can be used to obtain the total sum of squares (*SS_{total}*) through Equation 1 and
112 *BD_{Phy}* and *BD_{Fun}* by applying Equation 2.

$$113 \quad SS_{total} = \frac{1}{n} \sum_{h=1}^{n-1} \sum_{i=h+1}^n \mathbf{Dp}_{hi}^2 \text{ or } \mathbf{Df}_{hi}^2 \quad \text{Equation 1}$$

$$BD_{Phy} \text{ or } BD_{Fun} = \frac{SS_{total}}{n-1} = Var(\mathbf{P} \text{ or } \mathbf{X}) \quad \text{Equation 2}$$

The components that represents the phylogenetic and functional local contributions of each community, PLCBD and XLCBD respectively, can be obtained by using the algebra of principal coordinate analysis by computing matrix $\mathbf{A}$ ($-0.5 * D_{hi}^2$) and centering it to obtain matrix $\mathbf{G}$ through Equation 3. In equation 3, $\mathbf{1}$ is a vector of ones and $\mathbf{1}'$ its transposition.

$$\mathbf{G} = (\mathbf{I} - \frac{\mathbf{1}\mathbf{1}'}{n})\mathbf{A}(\mathbf{I} - \frac{\mathbf{1}\mathbf{1}'}{n}) \quad \text{Equation 3}$$

The diagonal elements of matrix $\mathbf{G}$ are SS_i values. Thus, dividing each value in the diagonal of $\mathbf{G}$ by SS_{total} we can obtain a measure that indicates the proportion that each sample unit accounts for of the total variation presented in $\mathbf{P}$ or $\mathbf{X}$ (PLCBD and XLCBD, respectively) (Equation 4).

$$PLCBD_i \text{ or } XLCBD_i = diag(\mathbf{G})/SS_{total} \quad \text{Equation 4}$$

More details on how to decompose BD into its components are provided by Legendre and De Cáceres (2013). The contribution of each species to total β -diversity can only be obtained when using calculations directly on matrices $\mathbf{P}$ and $\mathbf{X}$. Thus, we show here only the components of BD_{Phy} and BD_{Fun} associated with the local contribution of communities. Both PLCBD and XLCBD, like LCBD, can be interpreted as measures of community uniqueness regarding clade and functional composition, respectively. Appendix S1 of the Supplementary Material shows how the BD framework can be extended by directly using matrices $\mathbf{P}$ and $\mathbf{X}$ to obtain BD_{Phy} and BD_{Fun} , respectively, and all of their components (raw data approach). Figure S1 of the Supplementary Material illustrates how XLCBD and PLCBD can be interpreted using a simple example of a hypothetical metacommunity.

137 *A simulation-based evaluation of BD_{Phy} and BD_{Fun} as measures of phylogenetic and*
 138 *functional β -diversity*

139 We performed a set of simulations to assess the performance of BD_{Phy} , BD_{Fun} and their
 140 respective components, PLCBD and XLCBD, in capturing variation in phylogenetic
 141 and functional structure of metacommunities. The simulation procedure is based on the
 142 protocol proposed by Peres-Neto et al. (2012) (see also Minchin, 1987 for the original
 143 simulation approach), and allows the integration of phylogenetic relationships, species
 144 traits, species composition and environmental gradients in different ways to determine if
 145 the distribution of attributes of species and clades across communities mediate variation
 146 in metacommunity composition in a simulated environmental gradient. The procedure
 147 starts with a simulation of a phylogenetic tree and species traits. The presence of a
 148 species in a community is determined by a probability function that corresponds to a
 149 match between a species trait value and a simulated environmental value for each
 150 community.

151 We simulated four scenarios to test the performance (type I error and power) of
 152 the new metrics obtained using the expanded framework for β -diversity: (1)
 153 metacommunities in which phylogenetic and functional composition are responsible for
 154 variation in metacommunity composition (scenario W1,P1,X1); (2) metacommunities in
 155 which only clade composition is responsible for variation in metacommunity
 156 composition (scenario W1,P1,X0); (3) metacommunities in which only functional
 157 composition is responsible for variation in metacommunity composition (scenario
 158 W1,P0,X1); and, finally, (4) metacommunities in which neither clade distribution nor
 159 functional composition are responsible for variation in metacommunity composition
 160 (scenario W1,P0,X0).

161 To generate metacommunities according to scenario W1,P1,X1, we simulated a
 162 phylogenetic tree in which species presented traits with high phylogenetic signal, so that
 163 both trait and phylogenetic composition will vary across the metacommunity. In
 164 scenario W1,P1,X0, metacommunities were assembled from a phylogenetic tree in
 165 which species traits have phylogenetic signal, however, the trait used to calculate BD_{Fun}
 166 and XLCBD was not the same as the one used to assemble the metacommunity, thus,
 167 phylogenetic composition must show variation across the metacommunity, but not
 168 functional composition. In scenario W1,P0,X1, the metacommunities were assembled
 169 from a phylogenetic tree in which species did not present traits with phylogenetic
 170 signal, thus, functional composition will vary across the metacommunity, but not
 171 phylogenetic composition. Finally, in scenario W1,P0,X0, the metacommunities were
 172 assembled from a phylogenetic tree in which species traits did not present phylogenetic
 173 signal and the trait used to calculate BD_{Fun} and XLCBD was not the same as the one
 174 used to assemble the metacommunities, thus, neither functional nor distribution of
 175 clades were responsible for variation in composition across the metacommunity.

176 All metacommunities were simulated to possess 50 communities with species
 177 selected from a pool of 200. The simulation procedure was repeated 999 times for each
 178 scenario. Type I error and power for BD_{Fun} , BD_{Phy} , PLCBD and XLCBD were
 179 calculated by counting the number of times that the null hypothesis was rejected in each
 180 round of the simulation procedure. Each round consisted of: (1) simulating the
 181 phylogenetic tree, species traits and metacommunities; (2) calculating BD_{Phy} , BD_{Fun} and
 182 the local components PLCBD and XLCBD; (3) running a null model that deconstructs
 183 the original phylogenetic and functional relationships among species (taxa shuffle null
 184 model, Kembel et al., 2013) and recalculating BD_{Phy} , BD_{Fun} , PLCBD and XLCBD; (4)
 185 repeating step 3 three 999 times to assemble a null distribution of metrics; and (5)

186 comparing the observed values of BD_{Phy} and BD_{Fun} with the null distributions of BD_{Phy}
 187 and BD_{Fun} using $\alpha = 0.05$ as the nominal error to reject the null hypothesis. To test the
 188 performance of the metrics of local contribution, in step 4 we also obtained a F statistic
 189 from a linear model that related observed PLCBD and XLCBD with the environmental
 190 gradient used in the simulation and compared observed F with a null F distribution
 191 obtained from a linear model that relates the null PLCBD and null XLCBD with the
 192 environmental gradient. We compared the null F distribution with the observed F, also
 193 using the nominal $\alpha = 0.05$ to reject the null hypothesis (illustration of performance
 194 analysis is shown in Figure S3 of Appendix 2). More details on simulation procedures,
 195 models and theoretical expectations regarding PLCBD and XLCBD are presented in
 196 Appendix S2.

197 A summary of the four scenarios used to test the performance of the metrics
 198 proposed in this work is provided in Figure 2. Dimensions that presented variation in
 199 metacommunity composition in the simulation process are represented by the number
 200 one, while dimensions that did not mediate variation in the simulation process of the
 201 metacommunity are represented by a zero. Figure 2 also summarizes which scenarios
 202 were used to test power and which were used to test type I error. We did not perform
 203 tests of the original BD and LCBD since the statistical behaviors of these metrics were
 204 previously tested by Legendre and De Cáceres (2013). For more details about the
 205 simulation procedure and methods to obtain F values (models used to assess the
 206 performance of PLCBD and XLCBD) see Appendix S2 in Supplementary Material. We
 207 also tested the performance of all metrics proposed in this work using the raw data
 208 approach (Supplementary material).

209 *Empirical application: β -diversity of stream fish communities of a tropical river basin*

210 We illustrate how the new metrics proposed here can be used by calculating BD_{Phy} ,
 211 BD_{Fun} , PLCBD and XLCBD for tropical stream fish communities located in Brazil.
 212 This data comprises a sample of a metacommunity with 173 sites located in the
 213 Ivinhema River Basin, which is the main tributary of the Paraná River in the western
 214 part of the Paraná River Basin, one of the largest basins in South America. Each site
 215 corresponded to a stretch of approximately 100 meters in length and was sampled with
 216 the aid of an 80 x 120-cm rectangular sieve with a mesh size of 2mm. Electrofishing
 217 was also used at some sites.

218 We calculated BD, BD_{Phy} , BD_{Fun} and their local components, LCBD, PLCBD
 219 and XLCBD, for the 173 sampled sites. The BD metric was calculated using an
 220 incidence matrix standardized by the total occurrence of species in a community and
 221 subjected to a chord transformation. This standardization was done in order to keep BD,
 222 BD_{Phy} and BD_{Fun} on the same scale of variation. We assessed the significance of these
 223 metrics using two null models: site shuffle and taxa shuffle. Site shuffle randomizes
 224 species occurrence in the metacommunity by shuffling the lines of matrix **W**, with the
 225 rejection of the site shuffle null model ($\alpha \leq 0.05$) indicating that the composition of the
 226 community differs from that expected by chance. The taxa shuffle null model
 227 randomizes the tips of the phylogeny and functional dendrogram and uses these
 228 randomized structures to calculate, respectively, matrices **P** and **X**. The rejection of taxa
 229 shuffle indicates that the uniqueness of a community is also due to deep evolutionary
 230 relationships among the species or their functional attributes.

231 We performed a correlation analysis among LCBD, PLCBD and XLCBD using
 232 Pearson's correlation index, which allowed us to assess which dimensions serve as a
 233 proxy to indicate the local contribution of other dimensions. Finally, we represent the
 234 three quantities of local contribution spatially through an RGB plot to show how these

three components can be used together to identify sites of high importance regarding uniqueness. To generate the RGB plot we first standardize LCBD, PLCBD and XLCBD to vary between 0-250 and attribute to each combination of the three metrics a color in the gradient of RGB system. The redder the color the greater the uniqueness of a community regarding taxonomic composition; the greener the color the greater uniqueness regarding clade composition; the bluer the color the greater the uniqueness regarding functional composition. We also calculated how much each species contributed to β -diversity of Ivinhema River Basin regarding taxonomic (SCBD), phylogenetic (PSCBD) and functional (XSCBD) components (Appendix S4).

More details regarding the sampling design, the phylogenetic hypothesis and traits of the fish metacommunity used to calculate the metrics are provided in Nakamura et al. (2017) and Appendix S4. In Appendix S5 in Supplementary Material we provide the R function used to calculate all the metrics proposed in this work and for testing their significance according to the taxa shuffle null model (Kembel et al. 2013). We suggest that the distance metric to be used for the two metrics proposed here be the square root of Bray-Curtis index, which produces a maximum value of 0.5 for BD_{Phy} and BD_{Fun} for communities with completely different compositions. For the raw data procedure, we suggest the use of chord transformation of matrices **P** and **X** prior to the calculation of BD_{Phy} and BD_{Fun} metrics, which will produce values ranging from 0 to 1.

Results

Performance of metrics

We present here only the results of the simulation analysis for metrics calculated with the distance-based approach, while the results for the raw data approach are provided in Table S1 of Appendix S3 in Supplementary Material. **Error! Reference source not**

259 **found.** shows the statistical performance (rejection rate, type I error and power) for
 260 BD_{Phy} , BD_{Fun} , PLCBD and XLCBD, and the mean R^2 of the linear models relating the
 261 simulated environmental gradient to the metrics PLCBD and XLCBD, calculated for the
 262 four simulated scenarios. Both BD_{Phy} and BD_{Fun} had acceptable type I error values for
 263 all scenarios, with BD_{Phy} having a value of 0.05 for both W1,P0,X0 and W1,P0,X1, and
 264 BD_{Fun} presenting a probability of 0.04 for both W1,P0,X0, and W1,P1,X0. Similar
 265 results were found for the raw data approach, in which BD_{Phy} had values of 0.04 and
 266 0.05 in scenarios W1,X0,P0 and W1,X1,P1, respectively, whereas BD_{Fun} had values of
 267 0.05 for both W1,X0,P0 and W1,X0,P1 (Table S1 of Appendix S3 in Supplementary
 268 Material). Both BD_{Phy} and BD_{Fun} presented high values for power for all scenarios
 269 tested (ranging from 0.99 to 1).

270 PLCBD had a type I error rate of 0.04 in both W1,P0,X0 and W1,P0,X1,
 271 whereas XLCBD had type I error rates of 0.04 and 0.05 for W1,P0,X0 and W1,P1,X0,
 272 respectively. Both PLCBD and XLCBD had high rates of power ranging from 0.66 to 1.
 273 The lowest power value was obtained for PLCBD in scenario W1,P1,X1 for both the
 274 distance-based and raw data approaches (0.66 for both).

275 *Application of extended framework to stream fish communities.*

276 BD, BD_{Phy} and BD_{Fun} presented values of, respectively, 0.38, 0.09 and 0.01 for the
277 stream fish metacommunity of Ivinhema River Basin. BD_{Fun} and BD_{Phy} did not differ
278 significantly from expected values of the taxa shuffle null model (p-values > 0.05). The
279 contribution of local communities ranged from 0.003 to 0.009 for LCBBD and 0.002 to
280 0.02 for both PLCBD and XLCBD. Regarding uniqueness in composition, 23
281 communities presented significant values for the site shuffle null model for LCBBD, 26
282 for PLCBD and 45 for XLCBD. Of the 26 significant values for PLCBD, 11 were also
283 significant for taxa shuffle, indicating the effects of deep evolutionary relationships in
284 phylogenetic uniqueness of these communities. For XLCBD, 15 communities (from the
285 45 that presented significant p-values for site shuffle) presented significant values for
286 the taxa shuffle null model. Communities that presented significant values for PLCBD
287 and XLCBD for site and taxa shuffle are represented in Figure 3 by, respectively,
288 crossed circles and triangles.

289 All local components presented low correlation among each other, with the
290 highest correlation found being for LCBBD and PLCBD ($\rho = 0.46$; p-value < 0.001). This
291 lack of correspondence among components of local contribution can also be noted in
292 Figure 3. Figure 3 shows a predominance of a combination of low values for PLCBD,
293 XLCBD and PLCBD (circles with black color), indicating the predominance of
294 communities with low uniqueness. Only a few communities presented high values for at
295 least one component, with LCBBD being the component with more communities with
296 high uniqueness regarding taxonomic composition (represented by red circles). The
297 presence of high values for two components is even more rare among the communities
298 analyzed, indicating that is very rare for the communities of Ivinhema River Basin to

299 host unique species, clades or species that present very distinct attributes. In Appendix
300 S4 we also show the contribution of each species for Beta diversity of metacommunity.

301 **Discussion**

302 We demonstrated that the BD framework proposed by Legendre and De Cáceres (2013)
303 can be effectively extended to accommodate other components of biodiversity. The
304 extension presented here incorporates the advantages of the original BD framework
305 (decomposition into meaningful components of local and species contributions) while at
306 the same time effectively assessing β -diversity for phylogenetic and functional
307 dimensions of biodiversity, as shown by the performance analysis of the metrics.

308 As far as we are aware, the extension proposed in this work is the most general
309 in literature, since other propositions that seek to expand Legendre and De Cáceres´
310 framework lack some important characteristics presented in the original proposition.
311 Shooner et al. (2018) proposed a phylogenetic informed LCBD (also named as PLCBD)
312 by using a phylogenetic distance matrix containing PhyloSor values (Bryant et al. 2009)
313 for calculating LCBD. Since the use of a phylogenetic distance matrix among sites only
314 allows BD to be decomposed into the local contribution component, it is not possible to
315 obtain the portion of BD that accounts for species contribution to the total variation of
316 the metacommunity (SCBD component). The use of the fuzzy weighting method
317 together with Legendre and De Cáceres´ equations allows phylogenetic and functional
318 informed BD and all of its components to be derived, since the calculations can be made
319 using both distance and raw data approaches (using directly matrix **P** or **X**). Besides the
320 generality presented in our extension, we also highlight its flexibility, to obtaining new
321 β -diversity measures that capture other dimensions of biological diversity. For example,
322 a matrix containing genetic distances among species can be used in fuzzy-weight
323 transformation to obtain the genetic composition of sites (e.g. see Duarte et al., 2018),

324 which in turn can be used to compute a genetic informed BD measure and its
325 components. Therefore, the method presented here can be viewed as a unified approach
326 that allows the derivation of a family of β -diversity metrics with the same mathematical
327 characteristics yet encompassing different components of biological diversity.

328 The new local component metrics, PLCBD and XLCBD, can provide interesting
329 tools to address questions in the investigation of patterns of organization of
330 metacommunities. PLCBD can be used to identify patterns of variation present in the
331 phylogenetic structure of metacommunities related to sites that host clades with unique
332 evolutionary history. This information can be useful to test hypothesis that seek to
333 understand how the degree of phylogenetic uniqueness of sites is related to
334 environmental or historical factors (Graham & Fine, 2008; Leibold et al, 2010). Other
335 methods, like PCPS (Duarte, 2011), can also be used to identify distinct sites regarding
336 phylogenetic composition (heuristically, accompanied by an ordination procedure),
337 however, PLCBD offers a more direct assessment of community uniqueness together
338 with hypothesis testing to evaluate the role of species composition and deep
339 evolutionary relationships in generating observed patterns of phylogenetic uniqueness
340 (through site and taxa shuffle null models).

341 Regarding practical applications of PLCBD and XLCBD, we highlight their
342 utility for conservation purposes by identifying sites that deserve special attention due
343 to uniqueness in species composition, evolutionary history and functional attributes. In
344 this way they serve as complementary measures for studies that use local uniqueness
345 based solely from a taxonomic perspective (e.g. Landeiro et al. 2018). An integrative
346 approach that addresses multiple dimensions of variation in biological diversity can be
347 used to identify areas of congruence or mismatches in the distribution of biological

348 diversity, which can influence decisions made in conservation plans to preserve regional
349 biotas (Devictor et al. 2010; Meynard et al. 2011).

350 Our empirical example using a stream fish metacommunity illustrates how to
351 link patterns of variation in β -diversity related to taxonomic, phylogenetic and
352 functional diversity. Our findings complement those of Suárez et al (2011), by
353 evidencing that the processes influencing the distribution of species in the upper
354 Ivinhema River Basin are mainly mediated by variation in species composition and
355 contemporary environmental factors, with the deep evolutionary history of the species
356 having less impact on the structure of this metacommunity. By mapping LCBD,
357 PLCBD and XLCBD we can see that only a few sites possess unique compositions of
358 species, clades and attributes. Our multifaceted approach for beta diversity illustrates
359 how these three metrics can be used together to help identify areas of special
360 conservation interest (e.g., Devictor et al. 2010; Landeiro et al. 2018). The lack of a
361 spatial pattern in local contribution indicates that the communities have very similar
362 importance for the maintenance of the entire β -diversity of the Ivinhema River Basin.

363 *Concluding remarks and future directions*

364 We move forward in the operationalization of β -diversity patterns by presenting a
365 simple way to extend the BD framework in order to derive effective phylogenetic and
366 functional β -diversity measures. The methods used in this work to extend the original
367 framework are general enough to be used as a basis to obtain other metrics that can
368 represent other dimensions of biological diversity while at the same time preserve the
369 unique advantages presented in the original BD framework.

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376

377 Legends

378

379 Figure 1: Steps and numerical structures needed extend the BD framework for β -
 380 diversity. Solid boxes represent the original numerical structures presented in Legendre
 381 & De Cáceres (2013) to calculate BD, while dashed boxes comprise the matrices used
 382 in this paper to extend the original framework. The resemblance matrices $\mathbf{S}_f$ and $\mathbf{S}_p$ are
 383 necessary to obtain two matrices that describe communities by their trait ($\mathbf{X}$) and
 384 phylogenetic ($\mathbf{P}$) composition by means of fuzzy weighting. Distance matrices obtained
 385 from $\mathbf{P}$ and $\mathbf{X}$ are then used to obtain phylogenetic (PLCBD) or trait-based (XLCBD)
 386 measures of local contribution for beta diversity, respectively with the equations
 387 indicated in arrows.

388

389 Figure 2: Schematic representation of all simulation scenarios used to test the metrics
 390 proposed in this work. $\mathbf{W}$ represents a metacommunity that is generated by a simulation
 391 process, $\mathbf{P}$ and $\mathbf{X}$ represents functional and phylogenetic structure of metacommunity.
 392 When a given component of diversity presented variation in the metacommunity we
 393 assigned the number 1, on the contrary we attribute 0 in the table. The performance
 394 tested with each one of the scenarios (type I, power or both) is specified beside each
 395 scenario.

396

397 Figure 3: Map showing the distribution of LCBD, PLCBD and XLCBD values for fish
 398 communities of Ivinhema River Basin. Each point represents a combination of values of
 399 local contribution for the three dimensions. The redder the color the greater the
 400 uniqueness of a community regarding taxonomic composition; the greener the color the

401 greater uniqueness regarding clade composition; the bluer the color the greater the
402 uniqueness regarding functional composition. Communities that presented significant
403 values for PLCBD and XLCBD for site and taxa shuffle are represented by points with,
404 respectively, crossed circles and triangles.

405

406

407 **References**

- 408 Anderson MJ, Crist TO, Chase JM, et al (2011) Navigating the multiple meanings of
409 beta diversity: A roadmap for the practicing ecologist. *Ecol Lett* 14:19–28. doi:
410 10.1111/j.1461-0248.2010.01552.x
- 411 Baselga A (2010) Partitioning the turnover and nestedness components of beta
412 diversity. *Glob Ecol Biogeogr* 19:134–143. doi: 10.1111/j.1466-
413 8238.2009.00490.x
- 414 Bryant JA, Lamanna C, Morlon H, et al (2009) Microbes on mountainsides: Contrasting
415 elevational patterns of bacterial and plant diversity. *Light Evol* 2:127–148. doi:
416 10.17226/12501
- 417 Devictor V, Mouillot D, Meynard C, et al (2010) Spatial mismatch and congruence
418 between taxonomic, phylogenetic and functional diversity: The need for integrative
419 conservation strategies in a changing world. *Ecol Lett* 13:1030–1040. doi:
420 10.1111/j.1461-0248.2010.01493.x
- 421 Duarte LDS (2011) Phylogenetic habitat filtering influences forest nucleation in
422 grasslands. *Oikos* 120:208–215. doi: 10.1111/j.1600-0706.2010.18898.x
- 423 Duarte LDS, Debastiani VJ, Freitas AVL, Pillar VD (2016) Dissecting phylogenetic
424 fuzzy weighting: theory and application in metacommunity phylogenetics.
425 *Methods Ecol Evol* 7:937–946. doi: 10.1111/2041-210X.12547
- 426 Duarte LDS, Lima J de S, Maestri R, et al (2018) HaploVectors: an integrative
427 analytical tool for phylogeography. 1–21. doi: <https://doi.org/10.1101/330761>
- 428 Ellisson AM (2010) Partitioning diversity. *Ecology* 91:1988–1992. doi: 10.1890/09-
429 1692.1

- 430 Graham CH, Fine PVA (2008) Phylogenetic beta diversity□: linking ecological and
- 431 evolutionary processes across space in time. doi: 10.1111/j.1461-
- 432 0248.2008.01256.x
- 433 Kembel ASW, Ackerly DD, Blomberg SP, et al (2013) Package ‘ picante ’
- 434 Landeiro VL, Franz B, Heino J, et al (2018) Species-poor and low-lying sites are more
- 435 ecologically unique in a hyperdiverse Amazon region: Evidence from multiple
- 436 taxonomic groups. Divers Distrib 1–12. doi: 10.1111/ddi.12734
- 437 Legendre P, Borcard D, Peres-Neto P (2005) Analyzing Beta Diversity: Partitioning the
- 438 spatial variation of community composition data. Ecol Monogr 75:435–450
- 439 Legendre P, De Cáceres M (2013) Beta diversity as the variance of community data:
- 440 Dissimilarity coefficients and partitioning. Ecol Lett 16:951–963. doi:
- 441 10.1111/ele.12141
- 442 Leibold MA, Economo EP, Peres-Neto P (2010) Metacommunity phylogenetics:
- 443 Separating the roles of environmental filters and historical biogeography. Ecol Lett
- 444 13:1290–1299. doi: 10.1111/j.1461-0248.2010.01523.x
- 445 Li K, Liao M, Ni J, et al (2019) Treeline composition and biodiversity change on the
- 446 southeastern Tibetan Plateau during the past millennium, inferred from a high-
- 447 resolution alpine pollen record. Quat Sci Rev 206:44–55. doi:
- 448 10.1016/j.quascirev.2018.12.029
- 449 Meynard CN, Devictor V, Mouillot D, et al (2011) Beyond taxonomic diversity
- 450 patterns: How do α , β and γ components of bird functional and phylogenetic
- 451 diversity respond to environmental gradients across France? Glob Ecol Biogeogr
- 452 20:893–903. doi: 10.1111/j.1466-8238.2010.00647.x
- 453 Minchin PR (1987) Simulation of Multidimensional Community Patterns□: Towards a

- 454 Comprehensive Model. *Vegetatio* 71:145–156. doi: 10.1007/BF00039167
- 455 Nakamura G, Vicentin W, Suárez YR (2017) Functional and phylogenetic dimensions
- 456 are more important than the taxonomic dimension for capturing variation in stream
- 457 fish communities. *Austral Ecol* 1–11. doi: 10.1111/aec.12529
- 458 Peres-Neto P-R, Leibold M, Dray S (2012) Assessing the effects of spatial contingency
- 459 and environmental filtering on metacommunity phylogenetics. *Ecology* 93:14–30.
- 460 doi: 10.1890/11-0494.1
- 461 Pillar VD, Duarte LDS (2010) A framework for metacommunity analysis of
- 462 phylogenetic structure. *Ecol Lett* 13:587–596. doi: 10.1111/j.1461-
- 463 0248.2010.01456.x
- 464 Pillar VD, Duarte LDS, Sosinski EE, Joner F (2009) Discriminating trait-convergence
- 465 and trait-divergence assembly patterns in ecological community gradients. *J Veg*
- 466 *Sci* 20:334–348. doi: 10.1111/j.1654-1103.2009.05666.x
- 467 Safi K, Cianciaruso M V, Loyola RD, et al (2011) Understanding global patterns of
- 468 mammalian functional and phylogenetic diversity. *Philos Trans R Soc Lond B Biol*
- 469 *Sci* 366:2536–2544. doi: 10.1098/rstb.2011.0024
- 470 Shooner S, Davies TJ, Saikia P, et al (2018) Phylogenetic diversity patterns in
- 471 Himalayan forests reveal evidence for environmental filtering of distinct lineages.
- 472 *Ecosphere* 9:. doi: 10.1002/ecs2.2157
- 473 Whittaker RH (1960) Vegetation of the Siskiyou mountains, Oregon and California. *Ecol*
- 474 *Monogr* 30:279–338
- 475 Yao J, Zhang C, De Cáceres M, et al (2019) Variation in compositional and structural
- 476 components of community assemblage and its determinants. *J Veg Sci* 30:257–
- 477 268. doi: 10.1111/jvs.1270

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metacommunity simulation

W, P and X

W1,P1,X1
W1,P0,X1
W1,P1,X0
W1,P0,X0

BD	BD _{phy}	BD _{fun}	LCBD	PLCBD	XLCBD
1	1	1	1	1	1
1	0	1	1	0	1
1	1	0	1	1	0
1	0	0	1	0	0

1= variation
0= no variation

→ Power

Power and type I error