



**Interpreting the replacement and richness difference components of beta diversity**

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Interpreting the replacement and richness difference components  
of beta diversity

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## ABSTRACT

**Aim** The variation in species composition among sites, or beta diversity, can be decomposed into replacement and richness difference. A debate is ongoing in the literature concerning the best ways of computing and interpreting these indices. This paper first reviews the historical development of the formulas for decomposing dissimilarities into replacement, richness difference and nestedness indices. These formulas are presented using a unified algebraic framework, for species presence-absence and abundance. The indices decomposing beta play different roles in ecological analysis than beta diversity indices.

**Innovation** Replacement and richness difference indices can be interpreted and related to ecosystem processes. The pairwise index values can be summed across all pairs of sites; these sums form a valid decomposition of total beta diversity into total replacement and total richness difference components. Different communities and study areas can be compared: some may be dominated by replacement, others by richness/abundance difference processes. Within a region, differences among sites measured by these indices can then be analysed and interpreted using explanatory variables or experimental factors. The paper also shows that local contributions of replacement and richness difference to total beta diversity can be computed and mapped. A case study is presented involving fish communities along a river.

**Main conclusions** The different forms of indices are based upon the same functional numerators. These indices are complementary; they can help researchers understand different aspects of ecosystem functioning. The methods of analysis used in this paper apply to any of the indices recently proposed. Further work, based on ecological theory and numerical simulations, is required to clarify the precise meaning and domain of application of the different forms. The

forms available for presence-absence and quantitative data are both useful because these different data types allow researchers to answer different types of ecological or biogeographic questions.

## INTRODUCTION

Since Whittaker (1972), ecological dissimilarities have been used to measure beta diversity between sampling units. Koleff et al. (2002) reviewed 24 beta diversity indices proposed in the literature whereas Legendre & De Cáceres (2013) described 14 properties of 11 dissimilarity indices that are appropriate for beta diversity studies.

Harrison *et al.* (1992), Williams (1996) and Lennon *et al.* (2001) pioneered the idea that dissimilarities among communities result from two different processes: species replacement (also called turnover), and richness difference or nestedness (species gain and loss). Following these foundation publications, a series of papers (see Methods) appeared, proposing more refined or alternative ways of partitioning dissimilarity indices in beta diversity studies.

All authors use the same quantitative components, found when comparing community compositions at two sites ( $a$ ,  $b$ ,  $c$ ,  $(b + c)$ ,  $|b - c|$ ,  $\min(b, c)$ , Fig. 1), to construct replacement, richness difference and nestedness indices from species presence-absence data. Figures similar to Fig. 1 are found in several papers: Williams (1996), Baselga (2010, 2012), Podani & Schmera (2011) and Carvalho *et al.* (2013).

*Species replacement* refers to the well-known fact that species tend to replace each other along ecological gradients that are sufficiently long (e.g. Whittaker, 1952); the replacement rate is also a function of the ecological tolerance, or niche breadth, of the species. Species replacement is also called turnover when analyzed along spatial or environmental gradients. It implies the simultaneous gain and loss of species due to environmental filtering and historical

events (Leprieur *et al.*, 2011). The replacement component of dissimilarity measures (Appendix S1) may thus reflect the influence on community structure of the variables controlling ecological gradients.

*Richness difference* refers to the fact that a community may include a larger number of species than another. It may reflect the diversity of niches available at different locations along the sampling axis or throughout the study area. Differences in richness may be due to species thinning causing nestedness, or to other ecological processes.

*Nestedness* is a type of richness difference pattern characterized by the species at a site being a strict subset of the species at a richer site (Atmar & Patterson, 1993; Baselga, 2012). This is also the concept that underlies the nestedness indices of Podani & Schmera (2011). How to translate the concept of nestedness into an index is, however, a subject open to discussion as there is no unequivocal way to do it.

In the comparison of two sites, richness difference can be interpreted as nestedness *sensu stricto* only if the sites have ' $a$ ' species in common, with  $a > 0$ , and they differ in other species, one site being richer than the other. When  $a = 0$ , the richness difference between two sampling units cannot be interpreted as nestedness, which is logically 0 in that situation (Podani & Schmera, 2011; Carvalho *et al.*, 2013). In that case, the difference in species composition measured by dissimilarity indices is equal to species replacement plus richness difference, without reference to ecological processes producing nestedness. For real ecological data, replacement and richness difference (or nestedness) contribute jointly to the differentiation of the sites, and it is interesting to partition a dissimilarity matrix into these two components, which correspond to different ecological processes, provided that the components add up to the dissimilarity value (Fig. 1).

The first contribution of this paper is to review the historical development of the formulas proposed in the literature for decomposing dissimilarity indices into replacement, richness difference and nestedness indices. These formulas are casted into a unified algebraic framework, for species presence-absence and abundance data (Appendix S1).

The main contributions of this article are the following: (1) The paper demonstrates that the sums of the replacement and richness difference indices corresponding to all pairwise comparisons over a study area form a proper decomposition of the total beta diversity over that area. (2) It describes how the differences among sites measured by these indices can be analysed and interpreted using descriptive or experimental factors, or explanatory environmental variables. They can also be used to produce ordinations. (3) Finally, it shows how to compute local contributions of replacement and richness difference to total beta diversity. These contributions can be mapped to facilitate interpretation. The calculations are illustrated using an ecological case study. R software is presented in appendices.

## **METHODS**

Many papers appeared, mostly during the past four years, describing or discussing replacement, richness (or abundance) difference, and nestedness indices (Williams 1996; Lennon *et al.* 2001; Cardoso *et al.*, 2009; Baselga, 2010, 2012, 2013a; Podani & Schmera 2011; Schmera & Podani, 2011; Carvalho *et al.*, 2012, 2013; Podani *et al.*, 2013); index notations differed among papers. Because the present paper is limited in page space, a brief history of the development of these indices is presented in Appendix S1 together with a summary of the criticisms formulated against suggested indices.

That discussion shows that all authors agree on the dissimilarity coefficients that seem to be the most useful bases for decomposition: firstly, the Jaccard ( $D_J$ ) and Sørensen ( $D_S$ ) indices for presence-absence data, which are usually expressed in terms of the following quantities found in a contingency table crossing two vectors of presence-absence data:  $a$  = number of species present at both sites,  $b$  = number of species present at site 1 but not at site 2,  $c$  = number of species present at site 2 but not at site 1; secondly, the Ružička ( $D_R$ ) and percentage difference ( $D_{\%diff}$ ) dissimilarity coefficients for quantitative data. They also agree that the operational portion of the equations estimating replacement is the quantity  $\min(b,c)$  or  $2\min(b,c)$  used as the numerator of indices for presence-absence data and the quantity  $\min(B,C)$  or  $2 \times \min(B,C)$  used as the replacement numerator for quantitative data (meanings of  $B$  and  $C$ : see Appendix S1). For richness difference, the operational portion of the equations is  $|b - c|$  for presence-absence data; to estimate abundance difference for quantitative data, it is  $|B - C|$ .

#### Replacement, richness difference and nestedness indices

Appendix S1 describes the development of indices that decompose dissimilarity coefficients into replacement, richness/abundance difference and nestedness components. These indices belong to families that were developed by two groups of authors; for simplicity, they are called the Podani and Baselga families in this paper. Each family contains indices for species presence-absence and for abundance data. Both families were completed by new indices described in Appendix S1. The indices are designated as follows in this paper (formulas shown in Appendix S1, Table S1.1):

- Podani family, presence-absence data – Replacement indices:  $Repl_J$  and  $Repl_S$ , which are components of the Jaccard ( $D_J$ ) and Sørensen ( $D_S$ ) dissimilarities, respectively. Richness difference indices:  $RichDiff_J$  and  $RichDiff_S$ .

• Podani family, abundance data – Replacement indices:  $Repl_R$  and  $Repl_{\%diff}$ , which are components of the Ružička and percentage difference dissimilarities, respectively. Abundance difference indices:  $AbDiff_R$  and  $AbDiff_{\%diff}$ .

• Baselga family, presence-absence data – Replacement indices:  $Repl_{BJ}$  and  $Repl_{BS}$ , which are components of the Jaccard and Sørensen dissimilarities, respectively. Nestedness indices:  $Nes_{BJ}$  and  $Nes_{BS}$ .

• Baselga family, abundance data – Replacement indices:  $Repl_{BR}$  and  $Repl_{B\%diff}$ , which are components of the Ružička and percentage difference dissimilarities, respectively. Nestedness indices:  $Nes_{BR}$  and  $Nes_{B\%diff}$ .

From the exchanges that appeared in the recent literature, the following points are discussed in Appendix S1. This section only presents the conclusions reached in the appendix, where details are given.

• It is the numerators of the proposed indices that estimate replacement and richness difference. One can then scale the indices to values between 0 and 1 with denominators of one's choice, depending on the purpose of the study. The denominators of the Jaccard, Sørensen, Ružička and percentage difference dissimilarities, or those used by Baselga (2010, 2012) in his replacement (turnover) indices, can all be used. Ecologists should understand, however, that the chosen denominators might create distortions in the positioning of sites in an ordination, compared to using the numerator values only. None of the denominators proposed up to now have all the optimal qualities. The discussions about over- or under-estimation of species replacement by indices of the two families of indices are, actually, discussions about the choice of a denominator.



• The indices in the Podani family correspond to the concepts of replacement and richness/abundance difference. Those in the Baselga family are replacement (or turnover) and nestedness indices. Richness difference is not the same as nestedness. Podani & Schmera (2011) proposed an index of nestedness ( $N_{rel}$ ) that differs from their index of richness difference; they explained that the latter only represents a portion of nestedness. Hence the Baselga nestedness indices ( $Nes_{BJ}$  and  $Nes_{BS}$ ) should be compared to Podani & Schmera's relativized nestedness index, not to the richness difference indices of the Podani family ( $RichDiff_J$  and  $RichDiff_S$ ).

• In the two families, the replacement and richness difference (Podani family) or replacement and nestedness indices (Baselga family) sum to dissimilarity measures ( $D_J$ ,  $D_S$ ,  $D_R$ ,  $D_{\%diff}$ ). These four dissimilarities are appropriate for beta diversity assessment, following the criteria of Legendre & De Cáceres (2013). An important point is that the replacement, richness difference and nestedness indices are not themselves indices of beta diversity; they decompose dissimilarity coefficients that can be used to estimate beta diversity.

• Replacement and richness difference or nestedness indices should have an ecological interpretation. In that respect, indices in the Podani family are easy to interpret due to the logic of their construction. Likewise, interpretation of Baselga's replacement indices is clear, whereas that of his nestedness indices is more intricate, albeit logical.

• When matrices of indices are to be used to produce ordinations of the sites, the Podani-family richness/abundance difference indices ( $RichDiff_S$  and  $AbDiff_{\%diff}$ ) that decompose the Sørensen and percentage difference dissimilarities present clear advantages for ordination because the **RichDiff<sub>S</sub>** and **AbDiff<sub>%diff</sub>** matrices are Euclidean, meaning that the data points can be fully represented in Euclidean space by principal coordinate analysis (PCoA) without production of negative eigenvalues and complex ordination axes.

• Claims have been made that the *Repl* indices in the Podani family were correlated to species richness differences between the sampling units whereas indices in the Baselga family were not. Actually, all indices described in Appendix S1 do not depend directly (and linearly) on site richness since they can all be expressed without recourse to the richness of the compared sites,  $r_1$  and  $r_2$ . Section 6 of the appendix shows that they can all be expressed by equations containing only  $p_1$  and  $p_2$ , where  $p_1$  is the proportion of shared species in the first sampling unit,  $p_1 = a/r_1$ , and  $p_2$  is the proportion of shared species in the second sampling unit,  $p_2 = a/r_2$ ;  $a$  is the number of species in common between the two sites. Section 5 of the appendix shows an example where some replacement indices vary as an inverse function of richness difference and another example where they do not. Hence this criticism does not apply to any of the indices described in this paper.

#### Partitioning total beta diversity

Pelissier *et al.* (2003), Legendre *et al.* (2005) and Anderson *et al.* (2006) showed that the total variance of a community composition table is an appropriate measure of its variation in species composition, or beta diversity. Total beta can be directly computed from the community data table or from a dissimilarity matrix derived from it using an appropriate dissimilarity coefficient (Legendre & De Cáceres, 2013). Beta diversity can thus be computed as

$BD_{Total} = \sum_{h=1}^{n-1} \sum_{i=h+1}^n D_{hi}^2 / (n(n-1))$ . In that equation,  $\sum_{h=1}^{n-1} \sum_{i=h+1}^n D_{hi}^2 / n$  is the total sum of squares ( $SS_{Total}$ ); further division by  $(n-1)$  produces the total variance, or total beta diversity ( $BD_{Total}$ ).

For the  $D_S$  (Sørensen),  $D_J$  (Jaccard),  $D_{\%diff}$  and  $D_R$  dissimilarity coefficients, which are non-Euclidean, taking the square root of the dissimilarities makes the resulting matrices  $\mathbf{D}^{(0.5)} =$

197  $[D_{hi}^{0.5}]$  Euclidean (meaning described in the previous subsection; Legendre & Legendre, 2012,  
 198 Tables 7.2 and 7.3). For that reason, in the variance approach (previous paragraph), Legendre &  
 199 De Cáceres (2013) recommended, for these four coefficients, to take the square root of the  
 200 distances before computing total beta diversity,  $BD_{Total}$ :

$$201 \quad BD_{Total} = \sum_{h=1}^{n-1} \sum_{i=h+1}^n \sqrt{D_{hi}}^2 / (n(n-1)) = \sum_{h=1}^{n-1} \sum_{i=h+1}^n D_{hi} / (n(n-1)) \quad (1)$$

202 as shown by Whittaker (1972; Whittaker's formula gives twice the value of  $BD_{Total}$  produced by  
 203 eq. 1) and Legendre & De Cáceres (2013), where  $D_{hi}$  is the dissimilarity between sites  $h$  and  $i$ .

204 For any two sites  $h$  and  $i$ , in the Podani family of indices, replacement ( $Repl_{hi}$ ) plus richness  
 205 difference ( $RichDiff_{hi}$ ) is equal to  $D_{hi}$ . Likewise, in the Baselga family, replacement ( $Repl_{hi}$ ) plus  
 206 nestedness ( $Nes_{hi}$ ) is equal to  $D_{hi}$ . Hence, the sum of the  $Repl_{hi}$  plus the sum of the  $RichDiff_{hi}$   
 207 values is equal to the sum of  $D_{hi}$  values, and this relationship can be written:

$$208 \quad BD_{Total} = Repl_{Total} + RichDiff_{Total} \quad (2)$$

209 where

$$210 \quad Repl_{Total} = \sum_{h=1}^{n-1} \sum_{i=h+1}^n Repl_{hi} / (n(n-1)) \quad \text{and} \quad RichDiff_{Total} = \sum_{h=1}^{n-1} \sum_{i=h+1}^n RichDiff_{hi} / (n(n-1)).$$

211 Because these equations are similar to eq. 1, the quantities  $Repl_{Total}$  and  $RichDiff_{Total}$  form a true  
 212 partition of  $BD_{Total}$  for any community data matrix analysed using one of the four dissimilarity  
 213 functions considered in this paper. This allows ecologists to calculate the proportion of  $BD_{Total}$   
 214 accounted for by the replacement and richness (or abundance) difference fractions as

$$215 \quad Repl_{Prop} = Repl_{Total} / BD_{Total} \quad \text{and} \quad RichDiff_{Prop} = RichDiff_{Total} / BD_{Total} \quad (3)$$

216 The sum of  $Repl_{Prop}$  and  $RichDiff_{Prop}$  is 1. The denominators of the terms in these ratios,  $n(n-1)$ ,  
 217 cancel out and the proportions can be computed as

$$218 \quad Repl_{Prop} = \sum_{h=1}^{n-1} \sum_{i=h+1}^n Repl_{hi} / \sum_{h=1}^{n-1} \sum_{i=h+1}^n D_{hi} \quad (4a)$$

$$219 \quad \text{and } Rich_{Prop} = \sum_{h=1}^{n-1} \sum_{i=h+1}^n Rich_{hi} / \sum_{h=1}^{n-1} \sum_{i=h+1}^n D_{hi} \quad (4b)$$

220 For a single pair of sampling units  $h$  and  $i$ ,  $n = 2$ , so that  $BD_{Total}$  for that pair is  $D_{hi}/2$ , which  
 221 can be partitioned into  $Repl_{Total} = Repl_{hi}/2$  and  $RichDiff_{Total} = RichDiff_{hi}/2$ .

222 While the replacement and richness difference components are required for detailed  
 223 gradient analysis, the  $Repl_{Total}$  and  $RichDiff_{Total}$  indices are useful to determine which of the two  
 224 processes dominates among the sampling sites under study.

225 Similar relationships can be computed for the replacement ( $Repl_{BJ}$ ,  $Repl_{BS}$ ,  $Repl_{BR}$ ,  
 226  $Repl_{B\%diff}$ ) and nestedness ( $Nes_{BJ}$ ,  $Nes_{BS}$ ,  $Nes_{BR}$ ,  $Nes_{B\%diff}$ ) components in the Baselga family of  
 227 indices. These global indices offer simple alternatives to the multiple-site indices proposed by  
 228 Baselga (2010, 2013b). For ecological interpretation, the interest of analysing pairwise  
 229 replacement and nestedness matrices, instead of multiple-site indices, will be shown in the  
 230 following subsections and in the Case study.

231 An R function is provided in Appendix S3 to compute all distance, replacement, richness  
 232 difference and nestedness matrices described in this paper, as well as the partitioning of total beta  
 233 diversity described in the present section.

## 234 Explaining *Repl* and *RichDiff* variation

235       When replacement and richness difference have been estimated for all pairs of sites in a  
 236 study, the next step is to test hypotheses of explanations for their variation. For the dissimilarity  
 237 matrices  $\mathbf{D}_J$ ,  $\mathbf{D}_S$ ,  $\mathbf{D}_R$  and  $\mathbf{D}_{\%diff}$ , which represent beta variation, the distance-based redundancy  
 238 analysis (db-RDA) method of Legendre & Anderson (1999) can be used to explain the variation  
 239 of the species data by canonical analysis. That method consists of the following steps: first, a  
 240 principal coordinate analysis (PCoA) of the dissimilarity matrix is computed; the principal  
 241 coordinates are then used as the response data in redundancy analysis (RDA) against a matrix of  
 242 explanatory variables. That method works best when the dissimilarity matrix is Euclidean; in that  
 243 case, all principal coordinate axes are real and they account together for the entire variation  
 244 represented by the dissimilarity matrix. As mentioned in the previous section,  $\mathbf{D}_J$ ,  $\mathbf{D}_S$ ,  $\mathbf{D}_R$  and  
 245  $\mathbf{D}_{\%diff}$  matrices are non-Euclidean, but taking the square root of the dissimilarities makes the  
 246 resulting matrices  $\mathbf{D}^{(0.5)} = [D_{hi}^{0.5}]$  Euclidean (meaning described above). Using the complete set of  
 247 principal coordinates computed from  $\mathbf{D}^{(0.5)}$  in redundancy analysis allows ecologists to select the  
 248 most interesting explanatory variables in a stepwise manner or test the effect of a given  
 249 explanatory variable or factor on the among-site variation in community composition.

250       In most instances, the replacement (**Repl**), richness/abundance difference and nestedness  
 251 matrices are not fully Euclidean even after taking the square root of the coefficients, although  
 252 square-rooting reduces in important ways the non-Euclidean component of these matrices that  
 253 shows up as negative eigenvalues and complex ordination axes (in Appendix S1, Table S1.4  
 254 shows that only the **RichDiff<sub>S</sub>** and **AbDiff<sub>%diff</sub>** matrices of the Podani family are fully Euclidean).  
 255 McArdle & Anderson (2001) described a way of correctly testing the significance of the  
 256 canonical relationship between a dissimilarity matrix  $\mathbf{D}$  and a set of explanatory variables when

257 **D** is non-Euclidean. The method, which is of course also valid for Euclidean matrices, consists in  
 258 computing the projector (or '*hat*') matrix

$$259 \quad \mathbf{H} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}' \quad (5)$$

260 where **X** is the matrix of explanatory variables. Matrix **H** is also used in multiple regression and  
 261 RDA. Then compute the Gower-centred matrix **G**, which is the first step of principal coordinate  
 262 analysis (PCoA, Gower, 1966) before eigenvalue decomposition:

$$263 \quad \mathbf{G} = \left( \mathbf{I} - \frac{\mathbf{1}\mathbf{1}'}{n} \right) \mathbf{A} \left( \mathbf{I} - \frac{\mathbf{1}\mathbf{1}'}{n} \right) \quad (6)$$

264 where  $\mathbf{A} = [a_{hi}] = [-0.5D_{hi}^2]$ . Use these matrices to construct the *F*-statistic of RDA as follows:

$$265 \quad F = \frac{\text{tr}(\mathbf{HGH})/m}{\text{tr}[(\mathbf{I} - \mathbf{H})\mathbf{G}(\mathbf{I} - \mathbf{H})]/(n - m - 1)} \quad (7)$$

266 where  $\text{tr}()$  is the trace operator which sums the diagonal values of a square matrix, **I** is an identity  
 267 matrix of the same size as **H**, *m* is the rank of **X** centred by columns, and *n* is the number of  
 268 observations. This statistic can be tested by permutation, as done by the demonstration function  
 269 in Appendix S4. This method improves upon the test originally proposed by Legendre &  
 270 Anderson (1999), which is approximate in the case of non-Euclidean dissimilarity matrices. It is  
 271 recommended to square-root the values in the **Repl**, **RichDiff**, **AbDiff** and **Nes** matrices before  
 272 this analysis in order to reduce their non-Euclideanarity.

### 273 Local contributions

274 Local contributions to beta diversity (LCBD indices) are comparative indicators of the  
 275 ecological uniqueness of the sites for their contributions to beta diversity (Legendre & De  
 276 Cáceres, 2013). In an ordination diagram by principal coordinate analysis, the sites with high

LCBD values are those found far from the multivariate centroid of the graphs; LCBD is actually the squared distance of a site to the data centroid, which is the point of origin of the multivariate graph.

Large LCBD values indicate sites that have strongly different species compositions compared to a mean site. For conservation biology, large LCBD values may indicate sites that have unusual species combinations and high conservation value, or degraded and species-poor sites that are good candidates for ecological restoration. They may also correspond to special ecological conditions or result from the effect of invasive species on communities. LCBD values can be mapped to facilitate interpretation, as shown in the Legendre & De Cáceres (2013) paper.

For readers interested in computational details, LCBD indices are the diagonal values of the Gower-centred matrix  $\mathbf{G}$  (eq. 6) computed during principal coordinate analysis of the dissimilarity matrix; each value is then divided by the total sum of squares of the data, which is the sum of the diagonal values of  $\mathbf{G}$ . Because of that division, the sum of LCBD values computed over all sites is 1. Several dissimilarity functions, for presence-absence or abundance data, are available to compute total beta diversity as well as LCBD indices (Legendre & De Cáceres, 2013).

Here the calculation of LCBD indices is extended to replacement and richness difference. These new LCDB indices,  $Repl_{LCBD}$  and  $RichDiff_{LCBD}$ , measure how exceptional each site is, when compared to the other sites, in terms of replacement or richness (or abundance) difference. In an ordination of the replacement or richness difference indices, the sites with high values of  $Repl_{LCBD}$  and  $RichDiff_{LCBD}$  are those that are far from the multivariate centroid of the graph. Like total beta LCBD,  $Repl_{LCBD}$  and  $RichDiff_{LCBD}$  are the diagonal values of the Gower-centred dissimilarity matrix computed during principal coordinate analysis of the **Repl** and **RichDiff**

matrices, divided by the total sum of squares of the matrix. An R function is provided in Appendix S5 to compute LCBD from a dissimilarity, replacement, or richness difference matrix. Note that  $Repl_{LCBD}$  and  $RichDiff_{LCBD}$  computed from  $D$  do not add up to LCBD indices computed from the dissimilarity matrix. That is because in each case, the LCBD indices measure the squared distance of the sites to the multivariate centroid in an ordination diagram, and the three ordinations have unrelated axes, despite the fact that the **Repl** and **RichDiff** matrices add up to the corresponding **D** matrix.

### Simplex analysis

Podani & Schmera (2011) and Podani *et al.* (2013) noted that  $Repl + RichDiff = D$  and that the similarity  $S = (1 - D)$ , which imply that  $S + Repl + RichDiff = 1$ . These authors proposed to represent the triplets of values  $\{S, Repl, RichDiff\}$  corresponding to a point in a triangular graph that they called an SDR-simplex; examples are shown in the Case study section. The sides of the triangle bear scales of similarity (bottom edge, with zero on the left), richness difference (left edge, with 0 at the top) and replacement (right edge, with 0 at the bottom). Each triplet of values represents the similarity  $S = 1 - D$  as well as the two components of  $D$ . If one of the three components is zero, the point is found on the edge where that component has the value 0; for example, if replacement is 0, the point is found along the bottom edge. If two components are equal, the point is found on a median that originates on one of the vertices and ends in the centre of the opposite edge; for example, if replacement and richness difference are equal (values between 0 and 0.5), the points are on the median that originates in the lower-right corner and ends in the centre of the richness difference edge. Podani and Schmera (2011) provided a series of examples that help familiarize oneself with the interpretation of SDR simplices.



## CASE STUDY

Freshwater fish were collected by Verneaux (1973) in the Doubs River, a tributary of the Saône that runs near the France-Switzerland border in the Jura Mountains in eastern France. In his paper, Verneaux proposed to use fish communities to characterize ecological zones along European rivers and streams. The data include fish community composition at 30 sites along the 453 km course of the river, the site geographic coordinates, and environmental data (source: <http://adn.biol.umontreal.ca/~numeralecology/numecolR/>). Twenty-seven species were captured and identified. No fish were caught at site 8, hence that site was excluded from the reanalyses made by Borcard *et al.* (2011) as well as here.

This data set exhibits a strongly nested structure along the first five sites in the headwaters of the river. For example, a single species is present at site 1, then 3, 4, 8 and 11 at sites 2 to 5 (Fig. 2c). Using the binary forms of the coefficients,  $D_S$  or  $D_J$ , this strong ecological gradient produced replacement values of 0 among these 5 sites because  $\min(b,c)$  was always 0; all differences were captured by the richness difference part of the dissimilarity  $D$ . Looking at the 29 sites, the fish community is dominated by richness difference, which accounts for 72% of total beta diversity measured through  $D_S$  or  $D_J$  ( $RichDiff_{Prop}$ ), compared to 28% for species replacement ( $Repl_{Prop}$ ). In the **Repl** and **RichDiff** matrices, 27 pairs of sites had richness difference values of 0 compared to 150 pairs that had replacement values of 0. With presence-absence data, richness difference of 0 occurs when all differences between sites are attributed to species replacement, so that  $b = c$  and hence  $|b - c| = 0$ .

Let us examine the graphs of the indices comparing sites 1–29 with site 30 located downstream, where richness is high (Fig. 2a). Site 30 was selected as the reference because it corresponds to the historical point of entry of the species into the river. Reading the graph from

right to left, richness differences (triangles) are null or very small up to site 17, except for sites 25 to 23, discussed a few sentences down. Thereafter, the values increase markedly towards site 1 upstream. Replacement values (squares) are also very small until about site 19, where they increase slowly up to site 15, after which they drop along the upper course of the river. The replacement (squares) and richness difference (triangles) indices sum to the Jaccard distances (circles, often hidden by the red triangles in the right-hand portion of the graph). The same observations can be made for this data set from the indices computed using the Ružička index, which is the quantitative form of the Jaccard dissimilarity (Fig. 2b). Sites 25 to 23 stand out as different (shaded areas in Fig. 2); these sites suffer from agricultural pollution and have impoverished fish communities compared to the sites down- or upriver. These three sites have high phosphate, nitrate and ammonium concentrations, low dissolved oxygen, and high biological oxygen demand.

Ward hierarchical clustering of the sites based upon the matrix of environmental variables showed a first division of the sites between the upper (sites 1 to 22) and lower courses of the river (sites 23 to 30). The lower course is characterized by lower altitude and higher water discharge, higher hardness and biological oxygen demand, and lower oxygen concentrations. A test of significance of the variation of the  $\mathbf{D}_J$ ,  $\mathbf{Repl}_J$  and  $\mathbf{RichDiff}_J$  matrices against a factor representing the upper and lower groups of sites was carried out to illustrate the test of significance (eq. 7) of the variation in these matrices by a factor, using the function in Appendix S4. Note that the indices derived from the community composition data subjected to the test are independent of the environmental data used in the cluster analysis that produced the factor. The binary factor significantly explained the variation between the two groups for  $\mathbf{D}_J$  and  $\mathbf{Repl}_J$  (p-values of 0.005 and 0.001 respectively after 999 random permutations), but not for  $\mathbf{RichDiff}_J$  (p-value of 0.943).

This result was expected from the ordinations shown in Appendix S6, where sites 1-22 are clearly separated from sites 23-30 in the replacement ordinations, but not in the richness difference ordinations (Figs. S6.1 and S6.2). Tests based upon the quantitative forms of the indices produced similar results.

Following that, the variation among sites in the upper course of the river only (sites 1 to 22) was studied in more detail using the environmental variables. In order to identify the environmental variables that best explained each index, a principal coordinate analysis of each of the Jaccard-based matrices (with indices square-rooted) was carried out, with Lingoes correction for the negative eigenvalues in the case of the **Repl<sub>J</sub>** and **RichDiff<sub>J</sub>** matrices; matrix **D<sub>J</sub><sup>(0.5)</sup>** was Euclidean and did not produce negative eigenvalues. The principal coordinates were used as input response variables into a forward selection procedure in RDA (function `forward.sel()` of R package `packfor`, Dray *et al.*, 2012). The selected explanatory variables were {slope, hardness, nitrate and O<sub>2</sub>} for **D<sub>J</sub>**, {O<sub>2</sub>} for **Repl<sub>J</sub>**, and {slope, hardness and nitrate} for **RichDiff<sub>J</sub>**. The tests of significance using principal coordinates corrected for negative eigenvalues were only approximate (McArdle & Anderson, 2001). An exact test of significance was then computed for each matrix and its set of explanatory variables, using the function in Appendix S4, which implements the *F*-test described in eq. 7 in a permutation testing procedure. The variation in the **D<sub>J</sub>**, **Repl<sub>J</sub>** and **RichDiff<sub>J</sub>** matrices explained by the selected environmental variables (those listed above) was highly significant in all cases (p-values = 0.001) with high values of  $R^2_{adj}$  of 0.36, 0.44 and 0.47 respectively. Thus the *Repl* and *RichDiff* components of the species variation were significantly related to different environmental variables.

LCBD indices were computed for the replacement and richness difference indices decomposing Jaccard dissimilarities. These indices are shown on schematic maps of the river in

Fig. 3. Results obtained using decomposition of the quantitative Ružička distances are nearly identical. Note that the *Replacement LCBD* and *Richness difference LCBD* indices show the most exceptional sites for each type of index separately. They do not allow researchers to determine the relative importance of the replacement and richness difference processes in the study; that information will be provided by triangular graphs (below).

- In a principal coordinate ordination of the *Repl<sub>J</sub>* matrix (Appendix S6, Fig. S6.1a), sites 11-15 and 23-25 were the farthest from the centroid of the ordination diagram when considering all ordination dimensions. As a consequence, high LCBD values for replacement (*Repl<sub>LCBD</sub>* index) were found at sites 11 to 15, which is a transition zone (sites located at intermediate altitudes, with strong slope, high oxygen concentration like the upper section, and water discharge like the next lower section) between the head section of the river and the more quiet sections downstream, and at the polluted sites 23-25 (Fig. 3a) which are exceptional because of their low species richness reflecting extreme ecological conditions.

- In a principal coordinate ordination of the *RichDiff<sub>J</sub>* matrix (Appendix S6, Fig. S6.1b), sites 1-3 and 23 were the farthest from the centroid of the ordination diagram. Hence, high LCBD values for richness difference (*RichDiff<sub>LCBD</sub>* index) were found at sites 1-3 and 23 (Fig. 3b). These sites had very small species richness (1 to 4 species) and were thus very different in richness from the other sites (Fig. 2c). Among the remaining sites on the map, site 29 has the highest LCBD (albeit smaller than sites 1-3 and 23) because it has the highest richness.

Triangular graphs were used to represent the pairwise indices in the  $\mathbf{S} = (1 - \mathbf{D})$ , **Repl**, **RichDiff** and **AbDiff** matrices using all algebraic forms described in this paper. Graphs of this type were recommended by Podani & Schmera (2011) and Podani *et al.* (2013) for interpretation of the *Repl* and *RichDiff* indices. The results for the Jaccard and Sørensen indices on the one hand

(Fig. 4a,b) and for the Ružička and percentage difference indices on the other hand (Fig. 4c,d), are very similar. The graphs show that the among-site variation is dominated by richness difference (mean points [large dots] along the *RichDiff* or *AbDiff* axis near 0.5 in Figs 4a and 4c, and near 0.4 in 4b and 4d, compared to lower mean values along the *Repl* axis), confirming the values found above for  $RichDiff_{Prop} = 72\%$  of total beta diversity versus 28% for  $Repl_{Prop}$ . Remember that these two statistics use the sum of the  $D$  values as their denominator (eq. 4a,b), and that sum is  $n(n-1)/2$  minus the sum of the  $S$  values used in the triangular plots. That is why the  $RichDiff_{Prop}$  and  $Repl_{Prop}$  statistics are larger than the means of *RichDiff* and *Repl* shown by large dots along the graph margins. Note also the many triplets (points in the triangular graphs) along the *Similarity* axis that have *Repl* values of 0.

## DISCUSSION

Several forms of replacement and richness difference indices have been described in the literature, and arguments have been presented about the way these indices should be computed and about their interpretation. The key papers are listed in the introduction of Appendix S1. Further work, based on ecological theory and numerical simulations, is required to clarify the precise meaning and the domain of application of the different forms of these indices, which are most likely complementary and should help researchers understand different aspects of ecosystem functioning.

The present paper focussed on two families of indices and used a unified algebraic framework for their computation. These indices have interesting properties: the numerators of the indices are chosen to estimate the ecological phenomena of interest (replacement and richness/abundance difference), and the denominators are added afterwards to normalize the

indices. The sum of the replacement and richness difference components is always equal to the corresponding dissimilarity, binary (Jaccard or Sørensen) or quantitative (Ružička or percentage difference). The indices react monotonically to species composition (presence-absence) or abundance gradients, as shown by numerical simulations. The R function provided with this paper allows readers to check empirically that when the quantitative indices are computed on presence-absence data, they produce the same results as the binary versions of the indices; that fact can also be checked algebraically.

Podani & Schmera (2011) found a logical advantage in the Jaccard-based indices where the denominator is the total richness,  $(a+b+c)$ , or its quantitative equivalent, but it is too early to rule out the Sørensen-based indices that have a different denominator. In the analysis of real data sets, little differences were found between the two sets of results and the correlation between the Jaccard-based and Sørensen-based indices was very high. This result was expected because the numerators of the indices are the same (Table S1.2).

In the Podani family, the indices decomposing  $D_S$  present an advantage for ordination because  $RichDiff_S$  is Euclidean. For triangular plots on the contrary, interpretation of the indices decomposing  $D_J$  is algebraically marginally simpler because the denominator is the total number of species in each pair of sites under study. By opposition, in indices decomposing  $D_S$ , the denominator gives double weight to the  $a$  fraction, and this moves the points in the simplex towards the lower-right corner of the plot.

Computing indices is a first step; interpreting their variation is the next necessary step. This paper described statistical tools and methods for the interpretation of these new indices. That is its main contribution. The paper showed that the replacement and richness difference indices can be summed over the study sites in an area, and the sums can be divided by the sum of the

corresponding distances. These ratios estimate the relative contributions of the two ecological processes to beta diversity over the study area. This is because, for the Jaccard, Sørensen, Ružička and percentage difference dissimilarities, which are non-Euclidean, the sum of all pairwise dissimilarities over a study area, divided by  $n(n - 1)$ , estimates the beta diversity of the area. Different communities in the same area, as well as a community of interest in different study areas, may be compared using these ratios. Some communities may be dominated by replacement processes, others by richness/abundance difference processes, and this gives ecologists insights into the influence of environmental variation on communities and the importance of species interactions.

The paper then showed that the portions of beta diversity represented by the **Repl** and **RichDiff** or **AbDiff** matrices could be analysed and interpreted with respect to explanatory factors or sets of environmental variables, using a  $F$ -test of significance designed for the analysis of non-Euclidean matrices in redundancy analysis. In the same spirit, Dobrovolski *et al.* (2012) conducted a macroecological study relating the ratios  $Ne_{BS}/D_S$ , averaged over the eight neighbours of each map grid cell of the New World (in the manner of Lennon *et al.* 2001), to cell age (time since glaciation), for different groups of vertebrates: amphibians, birds and mammals. Their results supported the hypothesis that the nestedness component of beta diversity is more important in areas affected by glaciations until recent times.

The case study illustrates how the calculations are done. The last methodological section showed that local contributions can be computed for the replacement and richness difference components of beta diversity, and that these contributions can be plotted on a map of the study sites. Again, the case study illustrates that point.

Should one use the presence-absence or the quantitative forms of the indices? That same question must always be answered as part of the process of choosing dissimilarity indices. Experience shows that binary dissimilarity coefficients produce interesting results when communities differ in the species complements composing them and partly harbour different species. Quantitative indices are clearly appropriate when the species are largely the same and the communities differ mostly by the abundances of their species (species composition). The former situation is expected from communities that are geographically far apart, hence the binary forms of the beta diversity component indices are likely to produce interesting results in studies carried out at broad spatial scales, whereas the abundance forms of the indices are likely to be preferable in studies carried out within small spatial extents, where species composition should differ mostly in the abundances of the species. For the comparison of communities that are so geographically distant that they do not share species, analyses based on groups of species with similar traits, e.g. species guilds, may bring about useful comparative information (e.g. Villéger *et al.*, 2013). The indices can also be modified to incorporate phylogenetic information about species relatedness (Leprieur *et al.*, 2012; Cardoso *et al.*, 2014).

Methodological issues should also be factored into the decision. Quantitative indices can be used only when the abundance assessments are based on appropriate sampling procedures and are comparable among sites. Biomass, or diameters at breast height (dbh) for trees, can be used instead of abundance data to compute quantitative dissimilarity indices and partition them into replacement and richness difference indices. Binary coefficients, although likely to produce coarser results, are the only choice when the data come from different sources, or have been collected by different researchers over long periods, or come from indirect sources like governmental reports, grey literature or museum collections. Palaeolimnologists analysing



sediment cores prefer in most studies to rely on species presence-absence data; their confidence in the numbers of individuals or pollen grains observed for the various species is low because these numbers may not reflect the quantitative structure of the ancient communities they are studying. Presence-absence data are also often the most reliable basis for comparison of distant areas in macroecological studies.

For species abundance data with lognormal distributions, researchers often log-transform the data before computing the percentage difference dissimilarity. For abundance data with less extreme distributions, the square root transformation is often used prior to ordination analysis. The same can be done before computing the Ružička dissimilarity. These data transformations shrink the differences caused by high abundance values and change the computed dissimilarities (Legendre & Legendre, 2012, section 7.7). A word of caution is in order about the effect of these variance-reducing transformations on the *Repl* and *AbDiff* indices. For abundance data, these indices are computed on an individual basis. Log-transformed data produce values of *Repl* and *AbDiff* indices that are intermediate between the results obtained with raw abundance and with binary data. Hence, the results are not equivalent to those obtained from raw abundance data and their ecological interpretation may differ. Further research, including simulation studies, is required about the effect of transformations on *Repl* and *AbDiff* indices.

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618

## SUPPORTING INFORMATION

Additional supporting information may be found in the online version of this article at the publisher's web-site.

**Appendix S1** Description and discussion of the replacement, richness difference and nestedness indices.

**Appendix S2** Simulations showing that the replacement (*Repl*) and richness/abundance difference (*RichDiff* and *AbDiff*) indices respond monotonically to species gradients.

**Appendix S3** R function to compute the Podani- and Baselga-family decompositions of the Jaccard or Sørensen groups into replacement and richness difference (or nestedness) components, for species presence-absence or abundance data.

**Appendix S4** R function to compute the dbRDA *F*-test of significance between response data represented by a Euclidean or non-Euclidean dissimilarity matrix and a matrix of explanatory variables, following McArdle and Anderson (2001).

**Appendix S5** R function to compute LCBD indices from a dissimilarity matrix (**D**) or from beta diversity component matrices (**Repl**, **RichDiff**, **AbDiff** or **Nes**).

**Appendix S6** Principal coordinate ordinations of the replacement and richness difference indices for the fish case study data.

## FIGURE LEGENDS

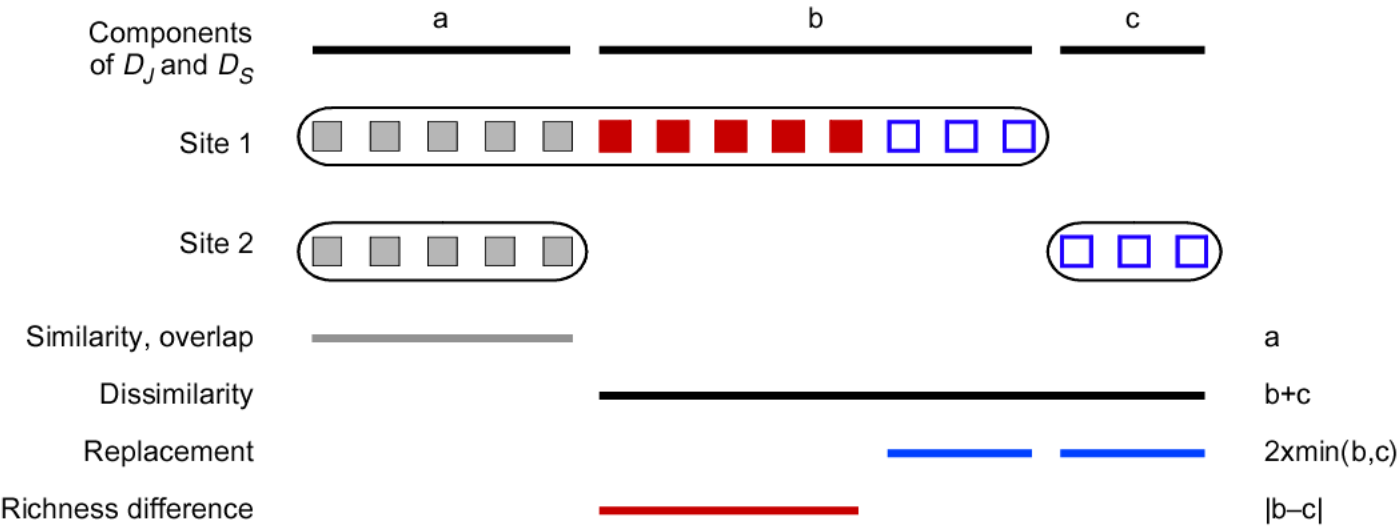
Figure 1 Comparison of species composition (16 species in total, squares) at two sites showing the components ( $a$ ,  $b$ ,  $c$ ) of the Jaccard ( $J$ ) and Sørensen ( $S$ ) dissimilarity coefficients for presence-absence data, and how these components are used to assess replacement (species with open squares) and richness difference (species with filled squares). Inspired from Williams (1996), Podani & Schmera (2011) and Carvalho *et al.* (2013). (Online version in colour.)

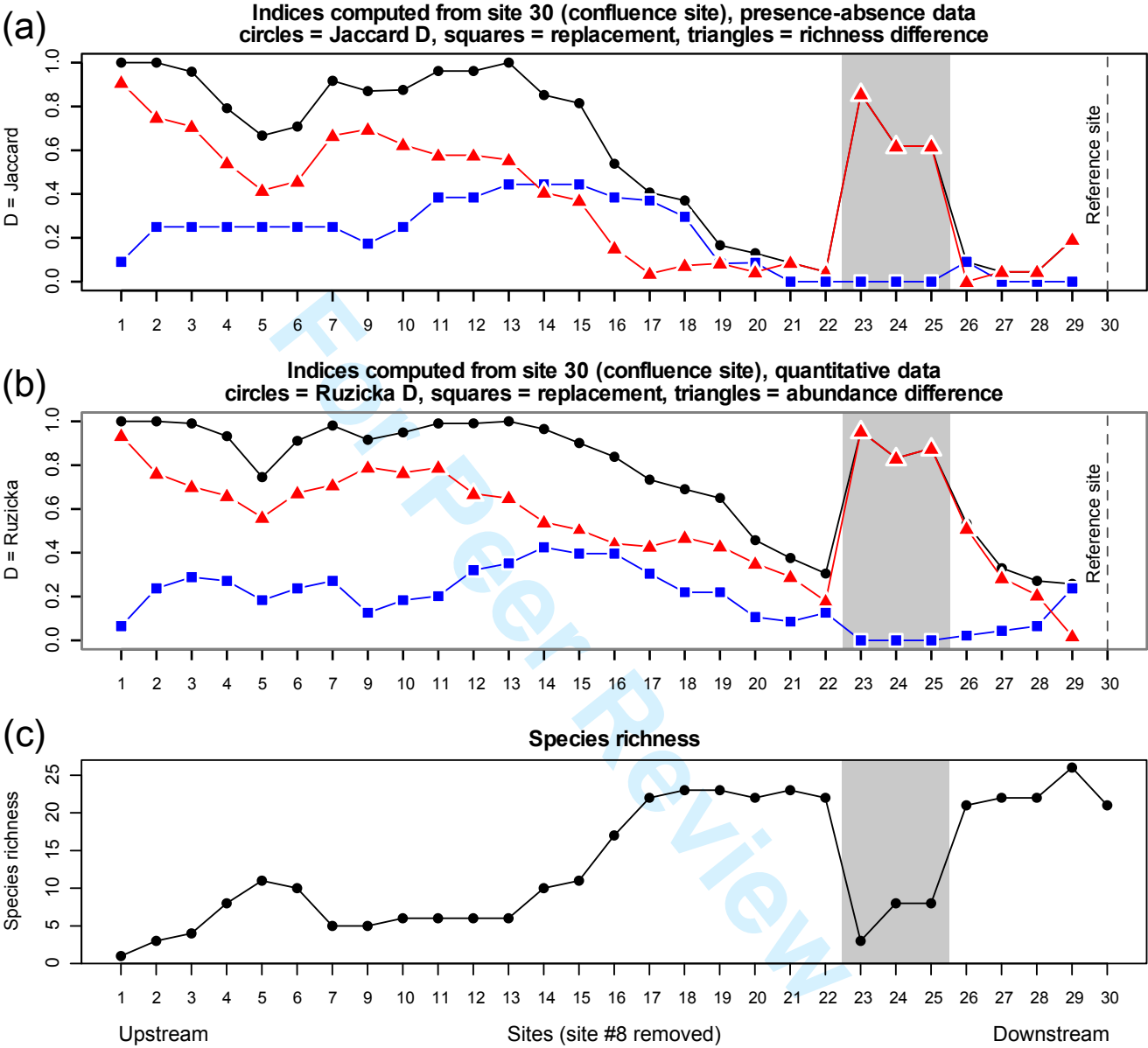
Figure 2 (a) *Jaccard dissimilarity* ( $D$ , circles), *Replacement* (squares) and *Richness difference* (triangles) indices for presence-absence data, comparing sites 1–29 with site 30. (b) Same, using species abundance data and the Ružička dissimilarity index. (c) Species richness at the study sites. The grey rectangles highlight sites 23 to 25 influenced by agricultural pollution. (Online version in colour.)

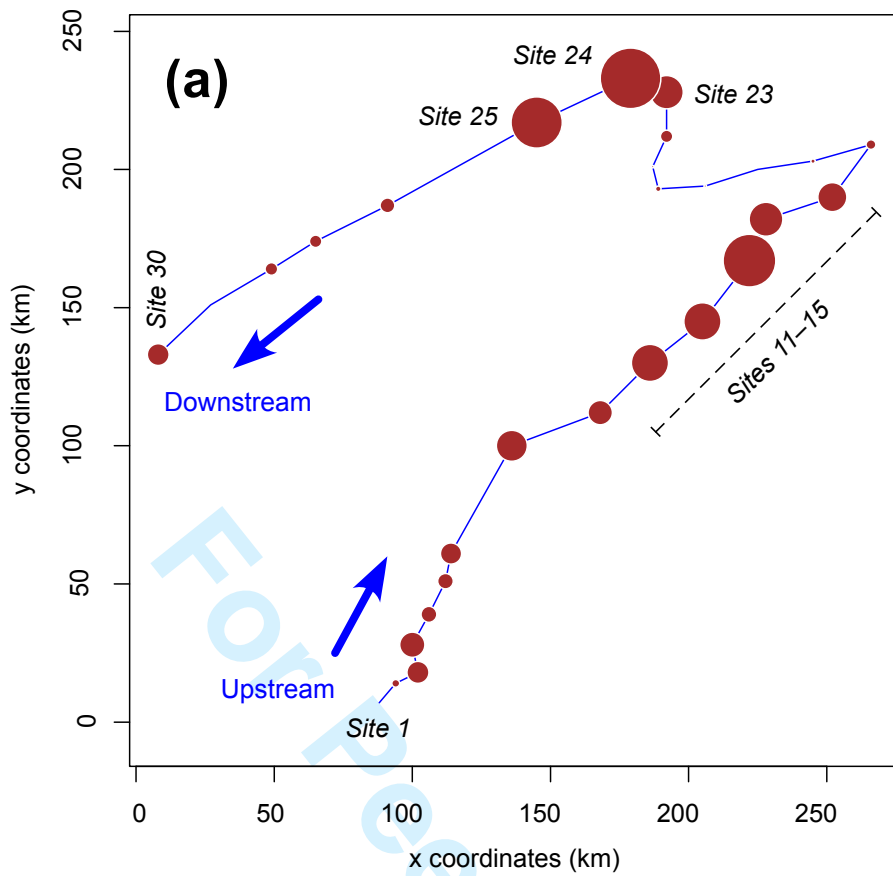
Figure 3 Schematic maps of Doubs River (line) showing the Podani-family (a) *Replacement LCBD* ( $Repl_{LCBD}$ ) and (b) *Richness difference LCBD* ( $RichDiff_{LCBD}$ ) of the binary fish assemblage data at the 29 study sites decomposing the Jaccard dissimilarity. Circle sizes are proportional to LCBD values. The arrows indicate water flow direction. (Online version in colour.)

Figure 4 Triangular plots (simplices) of the relationships among the 406 pairs of sites for the Doubs river fish data. Each point (black dot) represents a pair of sites. Its position is determined by a triplet of values from the  $\mathbf{S} = (1 - \mathbf{D})$  (similarity), **Repl** (replacement), **RichDiff** and **AbDiff** (richness and abundance difference) matrices; each triplet sums to 1. Graphs are shown for all algebraic forms of the Podani-family indices: (a) Jaccard, (b) Sørensen, (c) Ružička and (d) percentage difference. The large central dot in each graph (blue in the online version) is the centroid of the points; the smaller dots (blue in the online version) represent the mean values of the  $S$ ,  $Repl$  and  $Rich$  components.

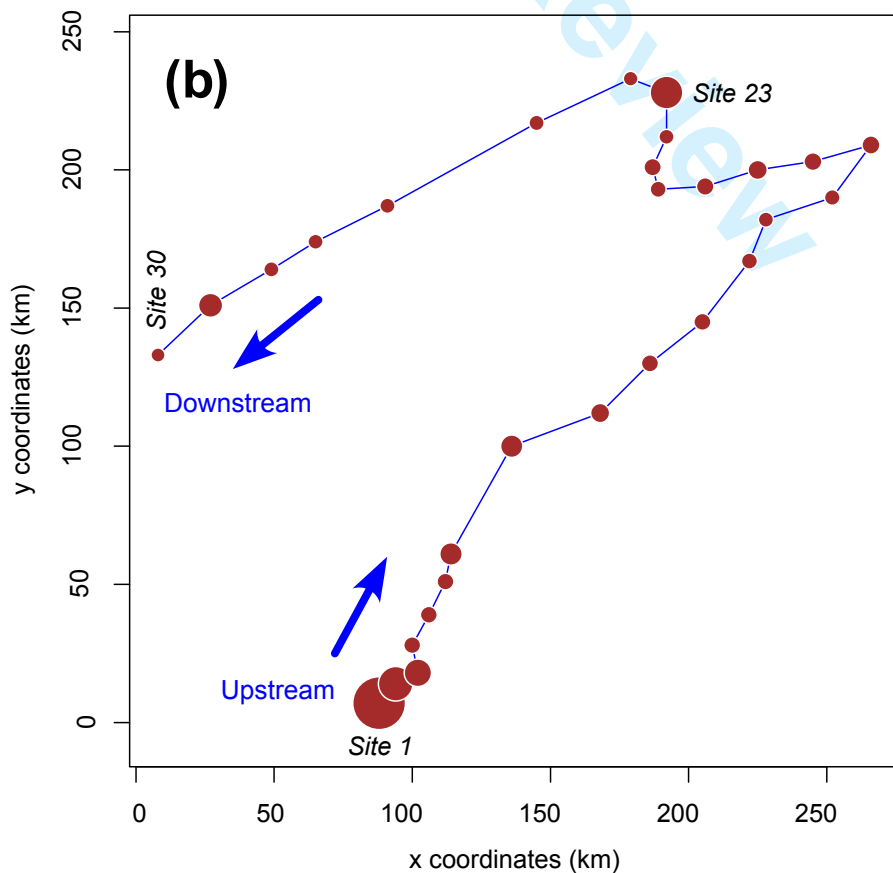




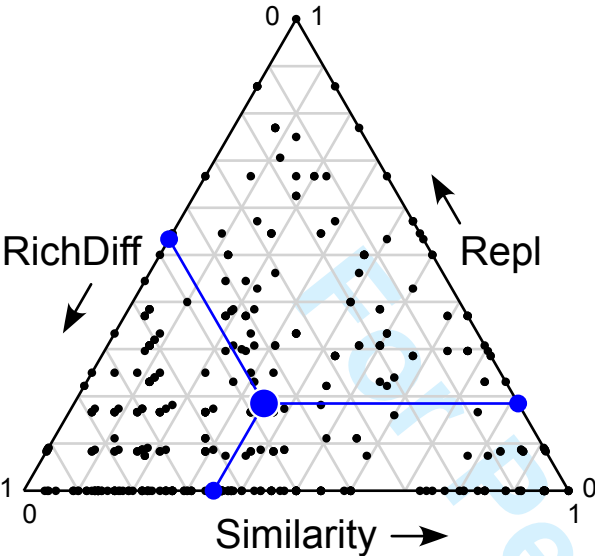




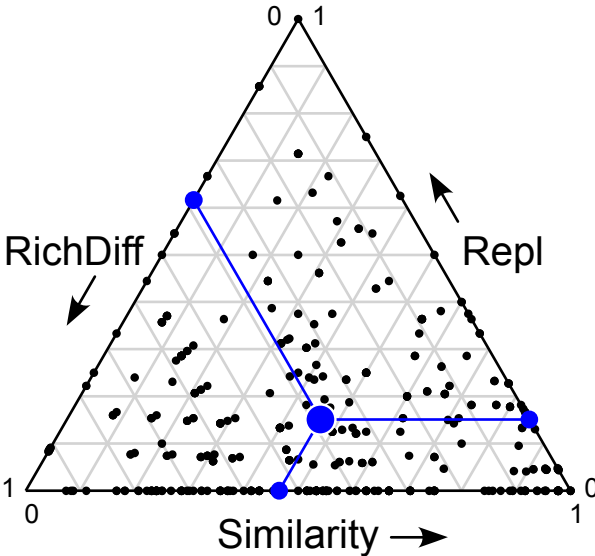
**Map of *Richness difference LCB***



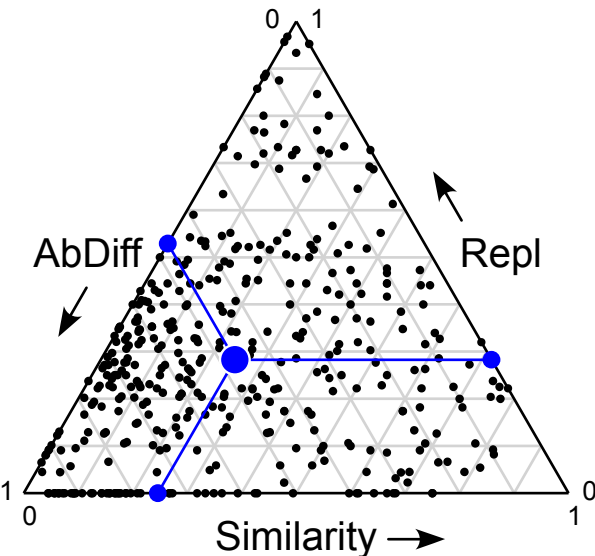
(a) Jaccard-based indices



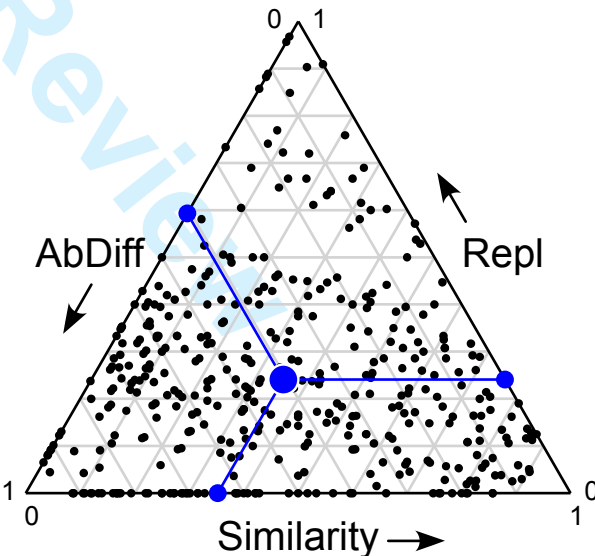
(b) Sørensen-based indices



(c) Ruzicka-based indices



(d) Percentage difference-based indices



*Appendix to:*

Legendre, P. Interpreting the replacement and richness difference components of beta diversity. *Global Ecology and Biogeography* (submitted).

## *Appendix S1*

### Replacement, richness difference and nestedness indices

#### **1. Introduction**

Whittaker (1960, 1972) described the alpha, beta and gamma diversity levels of natural communities. Alpha is local diversity, beta is spatial differentiation (or variation in species composition among sites), and gamma is regional diversity. Koleff *et al.* (2003) reviewed 24 beta diversity measures for species presence-absence data, reexpressed them in terms of the traditional  $a$ ,  $b$  and  $c$  values used for the comparison of pairs of sites, and classified them according to domains of application. This appendix focuses on some of these indices (Table S1.1) that are now used to estimate species replacement and richness difference, and are the subject of heated comparisons and discussions in the literature.

For species presence-absence data, two sites are compared using a 2×2 contingency table crossing the observed communities. The table contains the following frequencies:  $a$  = number of species present at both sites,  $b$  = number of species present at site 1 but not at site 2, and  $c$  = number of species present at site 2 but not at site 1. The number of species present at neither site,  $d$ , is also found in the contingency table, but it is not used in the calculation of the indices.

The two most widely used dissimilarity coefficients for presence-absence data are the Jaccard (1908;  $D_J = (b+c)/(a+b+c)$ ) and Sørensen (1948;  $D_S = (b+c)/(2a+b+c)$ ) indices. These coefficients have different mathematical properties:  $D_J$  is a metric whereas  $D_S$  is a semimetric (Legendre & Legendre, 2012). These dissimilarities can be partitioned into two components, the portions due to species replacement (*Repl* indices) and to either richness (*RichDiff*) or abundance difference (*AbDiff*), or nestedness (*Nes*); the corresponding concepts are discussed in the introduction of the main paper. Different forms of these indices have been proposed and can be computed from the values  $a$ ,  $b$  and  $c$ . Several papers appeared on the subject during the past years: Williams (1996), Lennon *et al.* (2001), Cardoso *et al.* (2009), Baselga (2010, 2012, 2013), Podani and Schmera (2011), Schmera & Podani (2011) and Carvalho *et al.* (2012, 2013) and Podani *et al.* (2013); index notations have also diverged among papers.

This brief historical account will focus on the contributions and indices that I consider the most important for users to understand how these indices are interrelated. The literature review is admittedly incomplete. It reflects personal choices from among the abundant literature published during the past few years on the subject.

#### *Early indices*

A first spatial turnover (or replacement) index was proposed by Williams (1996) who called it beta-3, meaning that it was the third modified form of Whittaker's (1972) famous  $\beta$

diversity index,  $\beta = \gamma/\alpha$ , where  $\gamma$  is regional richness and  $\alpha$  is the mean of the richness at individual sites. Williams applied the index to measure species turnover in small neighbourhoods of sampling units, e.g. quadrats. Koleff *et al.* (2003) labelled that index  $\beta_{-3}$  in their review paper on measures of beta diversity. Cardoso *et al.* (2009) modified the formula for  $\beta_{-3}$ , proposing to multiply the value by 2 to make it vary between 0 and 1; this is the current form of the  $\beta_{-3}$  index (Table S1.1).

A second replacement index was proposed by Lennon *et al.* (2001) who called it  $\beta_{\text{sim}}$ ; “sim” refers to palaeontologist G. G. Simpson, although  $\beta_{\text{sim}}$  differs from the asymmetric index used by Simpson to compare paleontological faunas in his 1943 paper. In similarity form, this index was applied by Lennon *et al.* (2001) to compare the community at a site to its eight first neighbours in a regular checkerboard grid of sampling units and compute the mean of these comparisons. Baselga (2010) based his first decomposition of  $D_S$  on  $\beta_{\text{sim}}$  (section 2.2).

Sections 2 and 3 describe the *Repl*, *RichDiff* or *AbDiff*, and *Nes* indices available in the recent literature for, respectively, species presence-absence and abundance data. The main paper shows how these indices can be interpreted and related to ecosystem functioning. *Repl*, *RichDiff*, *AbDiff* and *Nes* are new abbreviations introduced here to make the relationships among the indices easier to understand.

## 2. Replacement and richness difference indices: presence-absence data

### 2.1. Podani family

The indices proposed by Podani & Schmera (2011) and Carvalho *et al.* (2012, 2013), that expand upon Williams’ (1996) beta-3 index, are described first. For simplicity, these indices are referred to in this appendix as the Podani family. These authors suggested to estimate replacement (*Repl<sub>J</sub>*) as  $2 \times \min(b, c)$  and richness difference (*Rich<sub>J</sub>*) as  $|b - c|$ . These equations are justified by the test case illustrated in Fig. 1 of the main paper: three species of site 1 (represented by squares with positive-slope stripes, blue in the online version of the paper) are replaced by three species of site 2, whereas the richness difference (5 species represented by squares with negative-slope stripes, red in the online version,  $|b - c|$ ) is the remainder of the dissimilarity ( $b + c$ ) between the two sites. Because  $2 \times \min(b, c) = (b + c) - |b - c|$ , the sum of the replacement and richness difference values is equal to  $(b + c)$ , which is the numerator of the Jaccard dissimilarity coefficient ( $D_J$ , introduction section). Hence, if the replacement and richness difference indices are divided by the denominator of the Jaccard dissimilarity,  $(a + b + c)$ , the resulting scaled indices have a minimum value of 0 and a maximum of 1 and they sum to the Jaccard dissimilarity. The calculations are broken down into steps in Table S1.2. The resulting indices were called *relativized species replacement* ( $R_{\text{rel}}$ ) and *relativized richness difference* by Podani & Schmera (2011), and  $\beta_{-3}$  and  $\beta_{\text{rich}}$  by Carvalho *et al.* (2012, 2013).

Podani & Schmera (2011) also defined an index of nestedness:  $N = a + |b - c|$  if  $a > 0$  and  $N = 0$  if  $a = 0$ .  $N$  can be scaled to  $N_{\text{rel}}$  by division by  $(a + b + c)$ , which produces values in the range [0,1]. They clearly stated that nestedness is not the same as richness difference ( $|b - c|$ ).

Note that  $(b + c)$  is also the numerator of the Sørensen dissimilarity coefficient ( $D_S$ , introduction section). Carvalho *et al.* (2013) indicated that the replacement and richness difference indices could be divided by the denominator of the Sørensen dissimilarity,  $(2a + b + c)$ , although they did not find the resulting indices meaningful. Podani & Schmera’s (2011) view was

that one meaningful way of making the *Repl* and *RichDiff* indices independent of total species richness was to divide them by  $(a+b+c)$ ; see sections 5 and 6 (below) for a discussion of dependence/independence of species richness. With the  $(2a+b+c)$  denominator, the resulting standardized *Repl<sub>S</sub>* and *Rich<sub>S</sub>* indices now sum to the Sørensen dissimilarity (Table S1.2). This is a second, mathematically valid way of constructing indices. It satisfies Carvalho *et al.*'s (2013) first criterion for an ecologically meaningful way of partitioning beta diversity (Appendix S2).

Consider the following binary data example, which contains both a replacement and a richness difference component:

	Species 1	Species 2	Species 3	Species 4	Species 5
Site 1	1	1	1	0	1
Site 2	1	1	0	1	0

For these data,  $a = 2$ ,  $b = 2$  and  $c = 1$ ;  $2 \times \min(b, c) = 2$  (i.e. a species of Site 1 replaces a species of Site 2 and vice-versa);  $|b - c| = 1$  (i.e. after elimination of the two species involved in replacement, say species 3 and 4, species 5 is the only one showing richness difference);  $(a + b + c) = 5$ , and  $(2a + b + c) = 7$ . Hence,

- the Jaccard-based indices (*J*) are

$$Repl_J = 2 \times \min(b, c) / (a + b + c) \quad (R_{rel} \text{ in Podani \& Schmera 2011, } \beta_{-3} \text{ in Cardoso } et al. 2009) \quad (1)$$

$$Rich_J = |b - c| / (a + b + c) \quad (D_{rel} \text{ in Podani \& Schmera 2011}) \quad (2)$$

For the example data,  $Repl_J = 0.4$  and  $Rich_J = 0.2$ ; these values sum to  $D_J = (b + c) / (a + b + c) = 0.6$ .

- the Sørensen-based indices (*S*) are

$$Repl_S = 2 \times \min(b, c) / (2a + b + c) \quad (3)$$

$$Rich_S = |b - c| / (2a + b + c) \quad (4)$$

For the example data,  $Repl_S = 0.2857$  and  $Rich_S = 0.1429$ ; these values sum to  $D_S = (b + c) / (2a + b + c) = 0.4286$  (rounded values). So in each case, *Repl* and *RichDiff* add up to *D*.

Construction of indices for presence-absence data in the Podani family is summarized in Table S1.2.

## 2.2. Baselga family

Baselga (2010, 2012) described replacement and nestedness indices for species presence-absence data, calling the latter the *nestedness component* of dissimilarity indices. Baselga (2010) chose the  $\beta_{sim}$  index of Lennon *et al.* (2001) to estimate replacement because, according to these authors, that index clearly accounts for replacement (spatial turnover) and is only weakly correlated to the difference in species richness of the sites (but see section 6). He used  $\beta_{sim}$  in a more general way than Lennon *et al.* (2001) (see Introduction section), computing matrices of  $\beta_{sim}$  indices among all pairs of sites with the following formula:

$$Repl_{BS} = \beta_{sim} = \frac{\min(b, c)}{a + \min(b, c)} \quad (5)$$

( $Repl_{BS}$  in Table S1.3). Because the Sørensen dissimilarity  $D_S$  accounts for both replacement and nestedness, Baselga (2010) proposed to subtract  $\beta_{sim}$  from the Sørensen dissimilarity  $D_S$  to estimate the nestedness-resultant dissimilarity, or amount of dissimilarity derived from the nestedness component:

$$Nes_{BS} = \beta_{nes} = D_S - \beta_{sim} = \frac{|b - c|}{2a + b + c} \times \frac{a}{a + \min(b, c)} \quad (6)$$

( $Nes_{BS}$  in Table S1.3). Baselga (2010) offered the following interpretation for the algebraic form of that coefficient, whose meaning is not immediately clear: it is a measure of richness difference,  $|b - c|$ , divided by the denominator of  $D_S$ ; this part is also the Podani-family index  $Rich_S$ . The ratio is then multiplied (scaled) by the Simpson similarity  $(1 - \beta_{sim})$ ; if there are no species in common (i.e., if  $a = 0$ ), then  $\beta_{nes}$  is zero. This is a way of incorporating the constraint that nestedness is larger than 0 only if  $a > 0$ . That constraint is also found, in another algebraic form, in Podani & Schmera's (2011) nestedness index described above.

For the example data,  $Repl_{BS} = 0.3333$  and  $Nes_{BS} = 0.0952$ ; these values sum to  $D_S = (b + c)/(2a + b + c) = 0.4286$  (rounded values). The product extracts the difference in richness caused by nestedness from other types of richness differences (Baselga, 2010). Baselga did not consider his nestedness index to be a measure of richness difference.

Baselga (2012) proposed an alternative pair of indices designed to sum to the Jaccard dissimilarity  $D_J$ . He called the new turnover index  $\beta_{jtu}$  ( $Repl_{BJ}$  in Table S1.3) and the new nestedness index  $\beta_{jne}$  ( $Nes_{BJ}$  in Table S1.3):

$$Repl_{BJ} = \beta_{jtu} = \frac{2 \min(b, c)}{a + 2 \min(b, c)} \quad (7)$$

$$Nes_{BJ} = \beta_{jne} = D_J - \beta_{jtu} = \frac{|b - c|}{a + b + c} \times \frac{a}{a + 2 \min(b, c)} \quad (8)$$

For the example data,  $Repl_{BJ} = 0.5$  and  $Nes_{BJ} = 0.1$ ; the sum of these values is  $D_J = (b + c)/(a + b + c) = 0.6$ .

Construction of indices for presence-absence data in the Baselga family is summarized in Table S1.3.

### 3. Replacement and abundance difference indices: quantitative data

For presence-absence data, two sites that have the exact same species complement but differ in species abundances have replacement and richness difference values of 0 for coefficients  $D_S$  or  $D_J$  because  $b = c = 0$ . These 0 values are not informative of the quantitative differences that exist between the sites. The quantitative forms of the indices, described in this section, provide finer, more interpretable results when species abundance data are trustworthy.

Podani *et al.* (2013) and Baselga (2013) described ways of estimating replacement and richness difference based on species abundances, related to quantitative dissimilarities that are extensions of the Jaccard and Sørensen indices. Consider the following example:



	Species 1	Species 2	Species 3	Species 4	Species 5
Site 1	7	3	5	0	6
Site 2	2	4	0	3	0

Tamas *et al.* (2011) proposed the following notation to construct indices based on abundance data:  $A$  designates the sum of the minimum abundances of the various species, each minimum being the abundance at the site where the species is the rarest (this quantity is called  $W$  in Legendre & Legendre 2012, Chapter 7);  $B$  is the sum of abundances at site 1 minus  $A$ ; and  $C$  is the sum of abundances at site 2 minus  $A$ . The symbols have meanings similar to the lower-case letters  $a$ ,  $b$  and  $c$  used in the description of presence-absence indices:  $A$  is the sum of intersections (or the minima) of the abundances of the species at the two sites under comparison,  $B$  and  $C$  are the site-specific abundance complements. For the example data,  $A = 5$ ,  $B = 16$  and  $C = 4$ .

### 3.1. Podani family

In the context of quantitative community data, computation of the indices is individual-based instead of species-based. *Replacement* is easier to compute than to explain. For the site with the smallest total abundance (site 2 in the example), consider only the species (#2 and #4) that have larger abundances at that site than at site 1. Replacement refers to the fact that the individuals (4) that exceed the number of individuals of these species at site 1 are replaced, at site 1, by the same number (4) of individuals of different species. Replacement is computed as  $\min(B, C)$ ; this value is multiplied by 2 because the *replaced* and *replacing* individuals are both counted. Hence, replacement difference is  $2 \times \min(B, C)$ , which is  $2 \times 4 = 8$  for the example; computing this index for binary data produces the binary form of replacement,  $2 \times \min(b, c) = 2$ .

*Abundance difference* (abbreviated *AbDiff*) refers to the individuals that are not involved in replacement, that is, for the example,  $21 - 4 = 17$  individuals at site 1 and  $9 - 4 = 5$  individuals at site 2. The absolute value difference of these two values, 12, is the abundance difference. *AbDiff* can also be computed as the absolute value of the difference between  $B$  and  $C$ , which is  $|B - C| = 12$ . Again, computing this index for binary data produces the binary form of richness difference,  $|b - c| = 1$ .

What should we choose for denominator? The quantitative dissimilarity index of Ružička (1958) is one of the quantitative forms of the Jaccard index. Its formula is

$$D_R = (B + C) / (A + B + C) \quad (9a)$$

This coefficient can also be written as:

$$D_R = 1 - \left( \sum_{j=1}^p \min(y_{1j}, y_{2j}) / \sum_{j=1}^p \max(y_{1j}, y_{2j}) \right) \quad (9b)$$

$D_R$  computed for presence-absence data produces the Jaccard dissimilarity. As shown in Table S1.2,  $2 \times \min(B, C)$  (replacement) plus  $|B - C|$  (abundance difference) is equal to  $(B + C)$ . *Note* – There are other quantitative dissimilarity functions that correspond to the Jaccard index when applied to presence-absence data. Four are listed in Legendre & De Cáceres (2013, Table 1). However, none of those has the quantity  $(B + C)$  as its numerator, quantity that is the

sum of the replacement and abundance difference components; hence the choice of the Ružička index for the decomposition proposed by Podani *et al.* (2013).

Now if we apply the denominator of the  $D_R$  coefficient,  $(A + B + C)$  (eq. 9a), to the replacement and abundance difference numerators, we obtain  $Repl_R$  and  $Rich_R$  indices (Table S1.2):

$$Repl_R = 2 \times \min(B, C) / (A + B + C) \quad (10)$$

$$\text{and } AbDiff_R = |B - C| / (A + B + C) \quad (11)$$

Their sum is  $D_R$  (Table S1.2). For the example data,  $Repl_R = 0.32$  and  $AbDiff_R = 0.48$ , which sum to  $D_R = 0.80$ . Podani *et al.* (2013) described  $Repl_R$  as the *relativized abundance replacement index*,  ${}^aR_{\text{rel}(jk)}$ , and  $AbDiff_R$  as the *relativized abundance difference*,  ${}^aD_{\text{rel}(jk)}$ . For the example data,  $Repl_R = 0.32$  and  $AbDiff_R = 0.48$ , which sum to  $D_R = 0.80$ .

The quantitative dissimilarity that corresponds to the Sørensen index is the percentage difference ( $D_{\%diff}$ , Odum, 1950), incorrectly referred to by some authors as the Bray-Curtis index; see Legendre & De Cáceres (2013), footnote of their Table 1, about that story. The formula of that well-known dissimilarity index is

$$D_{\%diff} = (B + C) / (2A + B + C) \quad (12a)$$

Note that  $D_{\%diff}$  has the same numerator as  $D_R$ . The formula can also be written as (Odum, 1950):

$$D_{\%diff} = \sum_{j=1}^p |y_{1j} - y_{2j}| / \sum_{j=1}^p (y_{1j} + y_{2j}) = \sum_{j=1}^p |y_{1j} - y_{2j}| / (2A + B + C) \quad (12b)$$

where  $\mathbf{y}_1$  and  $\mathbf{y}_2$  are the two site vectors under comparison and  $p$  is the number of species in the data matrix (Legendre & Legendre, 2012, eq. 7.58). As mentioned above, the numerators of replacement and abundance difference (eqs. 10 and 11) sum to  $(B+C)$ , which is also the numerator of the  $D_{\%diff}$  index. Hence we can apply the denominator of the  $D_{\%diff}$  coefficient to these numerators to obtain  $Repl_{\%diff}$  and  $AbDiff_{\%diff}$  indices that sum to  $D_{\%diff}$  (Table S1.2):

$$Repl_{\%diff} = 2 \times \min(B, C) / (2A + B + C) \quad (13)$$

$$\text{and } AbDiff_{\%diff} = |B - C| / (2A + B + C) \quad (14)$$

The  $Repl_{\%diff}$  and  $AbDiff_{\%diff}$  indices do not seem to have been described in the literature yet and are thus new, although they stem from the same logic as the Podani *et al.* (2013) indices for quantitative data (eqs. 10 and 11). For the example data,  $Repl_{\%diff} = 0.2667$  and  $AbDiff_{\%diff} = 0.4000$ , which sum to  $D_{\%diff} = 0.6667$ .

Construction of indices for abundance data in the Podani family is summarized in Table S1.2.

### 3.2. Baselga family

Baselga (2013) described replacement and nestedness indices for species abundance data that sum to the percentage difference and correspond to the presence-absence indices described in his 2010 paper. He called the former *balanced variation component* and the latter *abundance gradient component* of dissimilarity indices. They are obtained by replacing the  $a$ ,  $b$  and  $c$

components of the indices for presence-absence data (eqs. 5 and 6) by the quantities  $A$ ,  $B$  and  $C$  defined above, which produces the following equations:

$$Repl_{B\%diff} = \frac{\min(B,C)}{A + \min(B,C)} \quad (15)$$

$$\text{and } Nes_{B\%diff} = \frac{|B - C|}{2A + B + C} \times \frac{A}{A + \min(B,C)} \quad (16)$$

For the example data,  $Repl_{B\%diff} = 0.4444$  and  $Nes_{B\%diff} = 0.2222$ , which sum to  $D_{\%diff} = 0.6667$ .

Replication and nestedness indices that sum to the Ružička dissimilarity can now be described. The  $Repl_{BR}$  and  $Nes_{BR}$  indices were not described by Baselga and are thus new.

$$Repl_{BR} = \frac{2\min(B,C)}{A + 2\min(B,C)} \quad (17)$$

$$\text{and } Nes_{BR} = \frac{|B - C|}{A + B + C} \times \frac{A}{A + 2\min(B,C)} \quad (18)$$

For the example data,  $Repl_{BR} = 0.6154$  and  $Nes_{BR} = 0.1846$ , which sum to  $D_R = 0.8000$ .

Construction of indices for abundance data in the Baselga family is summarized in Table S1.3.

All indices decomposing dissimilarities in the Podani and Baselga families, described above, have the property that when the quantitative indices are computed on presence-absence data, they produce the same results as the binary versions.

#### 4. Comparison of indices: which set of indices should one use?

During the past few years, arguments have been presented in favour or against each family of indices. Here is a short and possibly incomplete review of these exchanges.

##### 4.1. Richness difference versus nestedness

After the publication by Baselga (2010) of a first pair of indices ( $\beta_{sim}$  and  $\beta_{nes}$ ) decomposing  $D_S$ , Schmera & Podani (2011) argued that  $\beta_{nes}$  was simply the arithmetic difference between  $D_S$  and  $\beta_{sim}$ , without any connection to an ecological measure of species replacement or nestedness. They then summarised the partitioning of  $D_J$  into  $R_{rel}$  ( $Repl_J$ ) and  $D_{rel}$  ( $Rich_J$ ) described in Podani & Schmera (2011), where each component has clear ecological meaning, and they illustrated the differences between their indices and Baselga's using simulated and real ecological data. Baselga had explained, however, that  $\beta_{nes}$  was a *nestedness* index, whereas  $D_{rel}$  was defined by Podani & Schmera (2011) as a *richness difference* index. Podani & Schmera had recognized the difference between the two types of indices and defined a *nestedness* index ( $N$ ) associated with their  $R_{rel}$  ( $Repl_J$ ) and  $D_{rel}$  ( $Rich_J$ ) indices in their 2011 paper; see section 2.1

Baselga explained as follows the intricate formula of the nestedness index  $\beta_{nes}$ , which is the product of two components: "This product is needed to separate differences in richness caused by nestedness from other differences in richness" (Baselga 2010, p. 138). The difference between richness difference and nestedness is emphasized again in subsection 4.3 (below).

The Podani and Baselga families of decompositions have different objectives. In the Baselga family, dissimilarities are decomposed into turnover (or replacement) and nestedness components; the latter indices do not measure richness difference. In the Podani family, dissimilarities are decomposed into replacement and richness difference components; nestedness indices have also been proposed, but they are not an additive component of the dissimilarity indices. The message here is that these families of decompositions are not intended for the same purposes. They may be used to fulfil different objectives, and they may bring out complementary information when applied to the same data.

Among other criticisms that were voiced, Almeida-Neto (2012) criticized Baselga's  $\beta_{\text{nes}}$  on the ground that it did not behave like a true nestedness index because it did not satisfy the following conditions for selected simulated data: (1) it did not always increase when nestedness increased, (2) it should not have varied when nestedness remained constant, and (3) it should not have yielded positive values when there was no nestedness in the data.

#### 4.2. Over- or under-estimation of species replacement

The  $\beta_{\text{sim}}$  index of replacement ( $\text{Repl}_{BS}$ ) of Baselga was criticized by Carvalho *et al.* (2012) on the ground that it overestimated species replacement. Conversely, Baselga (2012) criticized Podani's  $\beta_{-3}$  index of replacement ( $\text{Repl}_J$ ) on the ground that it underestimated species replacement. *The difference in point of view is due to the denominator that serves as the reference in each index*; see formulas in Table S1.1. Podani & Schmera (2011) defined species replacement as  $R = 2 \times \min(b, c)$  without a denominator, indicating that it is the numerators of the proposed functions ( $\text{Repl}_J$ ,  $\text{Repl}_S$ ,  $\text{Repl}_{BJ}$ ,  $\text{Repl}_{BS}$ , all having the same numerator) that estimate replacement. One can then use the denominator of one's choice, depending on the purpose of the study. In the two families of indices, the replacement and richness difference (or nestedness) indices sum to dissimilarity measures ( $D_J$ ,  $D_S$ ,  $D_R$ ,  $D_{\%diff}$ ) that are all appropriate for beta diversity assessment, following the criteria of Legendre & De Cáceres (2013).

#### 4.3. Monotonicity

Carvalho *et al.* (2013) suggested that the replacement and richness difference indices should increase monotonically with increases in the amounts of replacement and richness difference in data. They carried out simulations using species presence-absence data. They found that the indices of Podani & Schmera (2011) that decompose  $D_J$  increased monotonically. That was not the case for Baselga's (2010, 2012)  $\beta_{\text{jne}}$  ( $\text{Nes}_{BJ}$ ) and  $\beta_{\text{nes}}$  ( $\text{Nes}_{BS}$ ), which are nestedness indices; results of simulations similar to those of Carvalho *et al.* (2013) are shown in Appendix S2, Fig. S2.2. I also computed the relativized nestedness index of Podani & Schmera (2011) for the simulated data; values of that index *decreased* monotonically with the amounts of replacement and richness difference. In any case, this is not a problem because these indices measure nestedness, not richness difference. According to Podani & Schmera (2011), the quantity  $|b - c|$ , which measures richness difference, does not fully reflect nestedness but only a contribution to it. Hence there is no constraining reason why nestedness indices should increase monotonically with increases in replacement and richness difference in data series.

I carried out further simulations to complete the picture. First, I verified that the indices of the Podani family that decompose  $D_S$  obeyed the monotonicity condition of Carvalho *et al.* (2013) (Appendix S2, Fig. S2.1). Then I carried out simulations using quantitative data to check that the quantitative indices developed by Podani *et al.* (2013) obeyed the monotonicity

condition. The results showed that the *Repl* and *AbDiff* forms of the Ružička and percentage difference indices reacted monotonically to gradual changes in quantitative community composition (Appendix S2, Fig. S2.3).

#### 4.4. Metric and Euclidean properties

Table S1.4 shows the metric and Euclidean properties of the dissimilarity coefficients ( $D_J$ ,  $D_R$ ,  $D_S$ ,  $D_{\%diff}$ ) and the corresponding *Repl* and *RichDiff*/*AbDiff*/*Nes* indices of the Podani (Table S1.4a) and Baselga (Table S1.4b) families. These properties are useful to select a coefficient to produce an ordination. The Jaccard and Ružička dissimilarities are metric whereas the Sørensen and percentage difference dissimilarities are semimetric. In all four cases, the dissimilarity matrix  $\mathbf{D}$  is not Euclidean but  $\mathbf{D}^{(0.5)} = [D_{hi}^{0.5}]$  is Euclidean (Legendre & Legendre, 2012, Table 7.2), meaning that the data points can be fully represented in Euclidean space by principal coordinate analysis (PCoA) without production of negative eigenvalues and complex ordination axes. In simple terms, they are fully appropriate for ordination by PCoA.

The Podani-family *RichDiff* indices decomposing the Sørensen (*RichDiff<sub>S</sub>*) and percentage difference (*AbDiff<sub>%diff</sub>*) indices present clear advantages for ordination over the *RichDiff<sub>J</sub>*, *AbDiff<sub>R</sub>* and *Nes* indices because the **RichDiff<sub>S</sub>**, **AbDiff<sub>%diff</sub>**, **RichDiff<sub>S</sub><sup>(0.5)</sup>** and **AbDiff<sub>%diff</sub><sup>(0.5)</sup>** matrices are metric and Euclidean. All other forms of indices are not metric nor Euclidean, so they should be subjected to corrections for negative eigenvalues when used to produce ordinations by principal coordinate analysis (Legendre & Legendre, 2012, section 9.3.4).

#### 4.5. Property P5 of Legendre & De Cáceres

Leprieur & Oikonomou (2014) argued that the Podani & Schmera (2011) measure of replacement  $\beta_{-3}$  lacked an important property that a dissimilarity measure should have when it is used in beta diversity studies, namely property P5 of Legendre & De Cáceres (2013), which states that *sites without species in common should have the largest dissimilarity*. For Legendre & De Cáceres (2013), that was indeed one of the important properties that should be fulfilled by dissimilarity coefficients used for beta diversity assessment. When we consider the pair *Repl<sub>J</sub>* and *Rich<sub>J</sub>*, or *Repl<sub>S</sub>* and *Rich<sub>S</sub>*, however, these indices are not used to measure beta diversity as a whole; they decompose the  $D_J$  and  $D_S$  dissimilarities that can be used to estimate beta diversity. It is  $D_J$  and  $D_S$  that should have property P5, not their components, and indeed they do. Replacement and richness difference indices are not used to carry out the same types of data analyses as dissimilarity indices; they have different purposes.

### 5. Artificial numerical examples

Leprieur & Oikonomou (2014) created an artificial data set to illustrate the fact that  $\beta_{-3}$  (*Repl<sub>J</sub>*) was correlated with differences in species richness between sites, whereas *Repl<sub>BJ</sub>*, ( $\beta_{jtu}$ ) and *Repl<sub>BS</sub>* ( $\beta_{sim}$ ) were not. That example is revisited here (Table S1.5). Only the first five sites of their example are used here. The data comparing the community of site A to those of sites B-E are presented in the form of the counts *a*, *b* and *c* used in the coefficient formulas (Table S1.1).

The replacement coefficients proposed by Baselga (2010, 2012), *Repl<sub>BJ</sub>* and *Repl<sub>BS</sub>*, are not correlated to richness difference in this example but *Repl<sub>J</sub>* and *Repl<sub>S</sub>* are negatively correlated to unscaled richness difference, *Rich.diff*.

Table S1.5. Coefficients and indices computed for the first artificial example. *Rich.diff*: unscaled richness difference computed as  $|b - c|$  or  $|r_1 - r_2|$ .  $r_1$ ,  $r_2$ ,  $p_1$ ,  $p_2$ : see text. Two dissimilarities:  $D_J$  (Jaccard) and  $D_S$  (Sørensen). Four replacement indices:  $Repl_{BJ}$ ,  $Repl_{BS}$ ,  $Repl_J$  and  $Repl_S$ ; four richness difference indices:  $Nes_{BJ}$ ,  $Nes_{BS}$ ,  $RichDiff_J$  and  $RichDiff_S$ .

(a) Coefficients									
Site pair	$a$	$b$	$c$	$r_1$	$p_1$	$r_2$	$p_2$	<i>Rich.diff</i>	
A-B	10	10	10	20	1/2	20	1/2	0	
A-C	10	10	20	20	1/2	30	1/3	10	
A-D	10	10	30	20	1/2	40	1/4	20	
A-E	10	10	40	20	1/2	50	1/5	30	

(b) Dissimilarity, replacement and richness difference indices											
Site pair	$D_J$	$D_S$	$Repl_{BJ}$	$Repl_{BS}$	$Repl_J$	$Repl_S$	$Nes_{BJ}$	$Nes_{BS}$	$RichDiff_J$	$RichDiff_S$	
A-B	0.667	0.500	0.667	0.500	0.667	0.500	0.000	0.000	0.000	0.000	
A-C	0.750	0.600	0.667	0.500	0.500	0.400	0.083	0.100	0.250	0.200	
A-D	0.800	0.667	0.667	0.500	0.400	0.333	0.133	0.167	0.400	0.333	
A-E	0.833	0.714	0.667	0.500	0.333	0.286	0.167	0.214	0.500	0.429	

Legendre & De Cáceres (2013, Appendix S3, property P10) showed, however, that  $D_J$  and  $D_S$  do not depend on the species richness,  $r_1$  and  $r_2$ , in the two sampling units that are compared;  $r_1 = a + b$  and  $r_2 = a + c$ . For proof, they showed that these dissimilarity coefficients can be expressed by formulas that do not contain  $r_1$  and  $r_2$  but only  $p_1$  and  $p_2$ , where  $p_1$  is the proportion of shared species in the first sampling unit,  $p_1 = a/r_1$ ; likewise,  $p_2$  is the proportion of shared species in the second sampling unit,  $p_2 = a/r_2$ . They considered this property P10 important for dissimilarity coefficients used for studying beta diversity; this property facilitates (although it does not ensure) the comparability of beta diversity values obtained for sampling units having different sizes or sampled using different efforts. That property can be demonstrated for all coefficients computed in Table S1.5 (see section 6 of the present Appendix): these coefficients are all invariant to the number of species in each sampling unit since they can be expressed by equations that only contain  $p_1$  and  $p_2$ .

The example in Table S1.5 had been tailored to support the claim of dependence of  $Repl_J$  and  $Repl_S$  on species richness  $r_2$ ; it does not show what happens when  $p_1$  and  $p_2$  remain constant across site comparisons. When they do, the ten coefficients produce constant values (i.e. they do

not change their values) when one changes  $r_1$  and  $r_2$  to any positive integer value under the constraint that  $r_1 p_1 = r_2 p_2$ .

To illustrate that property, a second example was generated using four pairs of unrelated sites (Table S1.6). In this example, the dissimilarity and replacement indices do not vary with changes in unscaled richness difference ( $Rich.diff = |b - c|$  or  $|r_1 - r_2|$ , last column in section (a) of the table), provided that  $r_1 p_1 = r_2 p_2 = a$ .

Table S1.6. Coefficients and indices computed for the second artificial example.

(a) Coefficients										
Site pair	$a$	$b$	$c$	$r_1$	$p_1$	$r_2$	$p_2$	$Rich.diff$		
A-B	3	9	3	12	0.25	6	0.5	6		
C-D	5	15	5	20	0.25	10	0.5	10		
E-F	10	30	10	40	0.25	20	0.5	20		
G-H	25	75	25	100	0.25	50	0.5	50		
(b) Dissimilarity, replacement and richness difference indices										
Site pair	$D_J$	$D_S$	$Repl_{BJ}$	$Repl_{BS}$	$Repl_J$	$Repl_S$	$Nes_{BJ}$	$Nes_{BS}$	$RichDiff_J$	$RichDiff_S$
A-B	0.800	0.667	0.667	0.500	0.400	0.333	0.133	0.167	0.400	0.333
C-D	0.800	0.667	0.667	0.500	0.400	0.333	0.133	0.167	0.400	0.333
E-F	0.800	0.667	0.667	0.500	0.400	0.333	0.133	0.167	0.400	0.333
G-H	0.800	0.667	0.667	0.500	0.400	0.333	0.133	0.167	0.400	0.333

In Table S1.6, the ten indices have identical values for all pairs of sites and they are totally unrelated to the unscaled richness difference between sites ( $Rich.diff$  column) since they are invariant. When the values of  $p_1$  and  $p_2$  do not change, the values of all indices do not change. The indices are related in highly nonlinear ways to the values of  $p_1$  and  $p_2$ , as shown by the equations in section 6. Data where the condition ( $r_1 p_1 = r_2 p_2 = a$ ) is violated may, of course, show correlations of  $Repl$  indices with richness difference on a case-by-case basis.

## 6. Proofs of property P10 for individual indices

Property P10 of Legendre & De Cáceres (2013) states the following:

*Indices for binary (species presence-absence) data that have this property do not directly depend on the number of species in the compared sampling units.*

Does the index value change if the two communities are species rich, compared to when the two communities are species poor or when one is rich and the other poor? Indices having property P10 do not change their values with changes in numbers of species  $r_1$  and  $r_2$ , in two sampling units  $\mathbf{x}_1$  and  $\mathbf{x}_2$  that are compared, provided that  $r_1 p_1 = r_2 p_2$ .

The following equalities and notations are used in the demonstrations:

- the total number of species (richness) in  $\mathbf{x}_1$  and  $\mathbf{x}_2$  are noted  $r_1 = a + b$  and  $r_2 = a + c$ ;
- the proportion of shared species with respect to the total richness at each site is  $p_1 = a/r_1 = a/(a + b)$  and  $p_2 = a/r_2 = a/(a + c)$ ;
- hence  $a = r_1 p_1 = r_2 p_2$ ,  $b = r_1(1 - p_1)$  and  $c = r_2(1 - p_2)$ .

The minimum of  $b$  and  $c$ , which we will need in the demonstrations, can be computed as  $\min(b, c) = ((b + c) - \text{abs}(b - c))/2 = (r_1(1 - p_1) + r_2(1 - p_2) - |r_1(1 - p_1) - r_2(1 - p_2)|)/2$

Also, because  $r_1 p_1 = r_2 p_2 = a$ , we have

- if  $r_1 > r_2$  then  $p_1 < p_2$ ; else if  $r_1 < r_2$  then  $p_1 > p_2$ ;
- $\min(b, c) = (r_1 + r_2 - 2r_1 p_1 - |r_1 - r_2|)/2 = (r_1 + r_2 - 2r_2 p_2 - |r_1 - r_2|)/2$ .

For the Jaccard and Sørensen similarity indices, demonstrations are provided in Appendix S3 of Legendre & De Cáceres (2013). The equations are reported again here, transformed into dissimilarities  $D_J$  and  $D_S$ .

Indices that have property P10 may still be empirically correlated (linearly or not) with differences in species richness for particular data sets.

### (1) Jaccard dissimilarity

$$D_J = 1 - \frac{1}{(1/p_1) + (1/p_2) - 1} = \frac{p_1 + p_2 - 2p_1 p_2}{p_1 + p_2 - p_1 p_2}$$

### (2) Sørensen dissimilarity

$$D_S = 1 - \frac{2}{(1/p_1) + (1/p_2)} = \frac{p_1 + p_2 - 2p_1 p_2}{p_1 + p_2}$$

These two dissimilarity coefficients are thus independent of  $r_1$  and  $r_2$ . The dissimilarity functions recommended in that paper for beta diversity studies all have property P10, but some other dissimilarity coefficients do not.

Following are the demonstrations for the replacement and richness difference indices, which all have property P10.

### (3) $\beta_{-3}$ or $Repl_J$ (Williams 1996, Podani & Schmera 2011)

$$\beta_{-3} = \frac{2 \min(b, c)}{a + b + c} = \frac{r_1 + r_2 - 2r_1 p_1 - |r_1 - r_2|}{r_1 p_1 + r_1(1 - p_1) + r_2(1 - p_2)} = \frac{r_1 + r_2 - |r_1 - r_2| - 2r_1 p_1}{r_1 + r_2 - r_2 p_2}$$



If  $r_1 > r_2$ , and considering that  $r_1 p_1 = r_2 p_2$ ,

$$\beta_{-3} = \frac{r_1 + r_2 - r_1 + r_2 - 2r_2 p_2}{r_1 + r_2 - r_2 p_2} = \frac{2r_2(1 - p_2)}{r_1 + r_2 - r_2 p_2}$$

Since  $r_1 = r_2 p_2 / p_1$ ,

$$\beta_{-3} = \frac{2r_2(1 - p_2)}{\frac{r_2 p_2}{p_1} + r_2 - r_2 p_2} = \frac{2r_2(1 - p_2)}{\frac{r_2 p_2}{p_1} + \frac{r_2 p_1}{p_1} - \frac{r_2 p_1 p_2}{p_1}} = \frac{2p_1(1 - p_2)}{p_1 + p_2 - p_1 p_2}$$

If  $r_1 < r_2$ ,

$$\beta_{-3} = \frac{r_1 + r_2 + r_1 - r_2 - 2r_1 p_1}{r_1 + r_2 - r_2 p_2} = \frac{2r_1(1 - p_1)}{r_1 + r_2 - r_2 p_2}$$

Since  $r_2 = r_1 p_1 / p_2$ ,

$$\beta_{-3} = \frac{2r_1(1 - p_1)}{r_1 + \frac{r_1 p_1}{p_2} - \frac{r_1 p_1 p_2}{p_2}} = \frac{2r_1(1 - p_1)}{\frac{r_1 p_2}{p_2} + \frac{r_1 p_1}{p_2} - \frac{r_2 p_1 p_2}{p_2}} = \frac{2p_2(1 - p_1)}{p_1 + p_2 - p_1 p_2}$$

Hence, considering that if  $r_1 > r_2$  then  $p_1 < p_2$ , or if  $r_1 < r_2$  then  $p_1 > p_2$ ,

$$\beta_{-3} = \frac{2 \min(p_1, p_2)(1 - \max(p_1, p_2))}{p_1 + p_2 - p_1 p_2}, \text{ which is independent of } r_1 \text{ and } r_2.$$

**(4) *Repl<sub>S</sub>*** (Carvalho *et al.* 2013)

$$Repl_S = \frac{2 \min(b, c)}{2a + b + c} = \frac{r_1 + r_2 - 2r_1 p_1 - |r_1 - r_2|}{2r_1 p_1 + r_1(1 - p_1) + r_2(1 - p_2)} = \frac{r_1 + r_2 - |r_1 - r_2| - 2r_1 p_1}{r_1 + r_2 + r_1 p_1 - r_2 p_2}$$

If  $r_1 > r_2$ , and considering that  $r_1 p_1 = r_2 p_2$ ,

$$Repl_S = \frac{r_1 + r_2 - r_1 + r_2 - 2r_2 p_2}{r_1 + r_2} = \frac{2r_2(1 - p_2)}{r_1 + r_2}$$

Since  $r_1 = r_2 p_2 / p_1$ ,

$$Repl_S = \frac{2r_2(1-p_2)}{\frac{r_2 p_2}{p_1} + r_2} = \frac{2r_2(1-p_2)}{\frac{r_2 p_2}{p_1} + \frac{r_2 p_1}{p_1}} = \frac{2p_1(1-p_2)}{p_1 + p_2}$$

If  $r_1 < r_2$ , and considering that  $r_1 p_1 = r_2 p_2$ ,

$$Repl_S = \frac{r_1 + r_2 + r_1 - r_2 - 2r_1 p_1}{r_1 + r_2} = \frac{2r_1(1-p_1)}{r_1 + r_2}$$

Since  $r_2 = r_1 p_1 / p_2$ ,

$$Repl_S = \frac{2r_1(1-p_1)}{r_1 + \frac{r_1 p_1}{p_2}} = \frac{2r_1(1-p_1)}{\frac{r_1 p_2}{p_2} + \frac{r_1 p_1}{p_2}} = \frac{2p_2(1-p_1)}{p_1 + p_2}$$

Hence, considering that if  $r_1 > r_2$  then  $p_1 < p_2$ , or if  $r_1 < r_2$  then  $p_1 > p_2$ ,

$$Repl_S = \frac{2\min(p_1, p_2)(1 - \max(p_1, p_2))}{p_1 + p_2}, \text{ which is independent of } r_1 \text{ and } r_2.$$

**(5)  $\beta_{jtu}$  (Baselga 2012) ( $Repl_{BJ}$  in this Appendix)**

$$\beta_{jtu} = \frac{2\min(b, c)}{a + 2\min(b, c)} = \frac{r_1 + r_2 - 2r_1 p_1 - |r_1 - r_2|}{r_1 p_1 + r_1 + r_2 - 2r_1 p_1 - |r_1 - r_2|} = \frac{r_1 + r_2 - |r_1 - r_2| - 2r_1 p_1}{r_1 + r_2 - |r_1 - r_2| - r_1 p_1}$$

If  $r_1 > r_2$ , and considering that  $r_1 p_1 = r_2 p_2$ ,

$$\beta_{jtu} = \frac{r_1 + r_2 - r_1 + r_2 - 2r_2 p_2}{r_1 + r_2 - r_1 + r_2 - r_2 p_2} = \frac{2r_2(1-p_2)}{2r_2(1-0.5p_2)} = \frac{1-p_2}{1-0.5p_2}$$

If  $r_1 < r_2$ ,

$$\beta_{jtu} = \frac{r_1 + r_2 + r_1 - r_2 - 2r_1 p_1}{r_1 + r_2 + r_1 - r_2 - r_1 p_1} = \frac{2r_1(1-p_1)}{2r_1(1-0.5p_1)} = \frac{1-p_1}{1-0.5p_1}$$

Hence, considering that if  $r_1 > r_2$  then  $p_1 < p_2$ , or if  $r_1 < r_2$  then  $p_1 > p_2$ ,

$$\beta_{jtu} = \frac{1 - \max(p_1, p_2)}{1 - \max(p_1, p_2)/2}, \text{ which is independent of } r_1 \text{ and } r_2.$$

**(6)  $\beta_{\text{sim}}$  (Baselga 2010) ( $Repl_{BS}$  in this Appendix)**

$$\beta_{\text{sim}} = \frac{\min(b,c)}{a + \min(b,c)} = \frac{(r_1 + r_2 - 2r_1p_1 - |r_1 - r_2|)/2}{r_1p_1 + (r_1 + r_2 - 2r_1p_1 - |r_1 - r_2|)/2} = \frac{r_1 + r_2 - |r_1 - r_2| - 2r_1p_1}{r_1 + r_2 - |r_1 - r_2|}$$

If  $r_1 > r_2$ , and considering that  $r_1p_1 = r_2p_2$ ,

$$\beta_{\text{sim}} = \frac{r_1 + r_2 - r_1 + r_2 - 2r_2p_2}{r_1 + r_2 - r_1 + r_2} = \frac{2r_2(1 - p_2)}{2r_2} = 1 - p_2$$

If  $r_1 < r_2$ ,

$$\beta_{\text{sim}} = \frac{r_1 + r_2 + r_1 - r_2 - 2r_1p_1}{r_1 + r_2 + r_1 - r_2} = \frac{2r_1(1 - p_1)}{2r_1} = 1 - p_1$$

Hence, considering that if  $r_1 > r_2$  then  $p_1 < p_2$ , or if  $r_1 < r_2$  then  $p_1 > p_2$ ,

$\beta_{\text{sim}} = 1 - \max(p_1, p_2)$ , which is independent of  $r_1$  and  $r_2$ .

**(7) Richness difference and nestedness indices**

Because the  $D_J$  and  $D_S$  dissimilarities and the four replacement indices obey P10, the corresponding richness difference indices must also have property P10. Indeed, the richness difference and nestedness indices are computed as a dissimilarity (either  $D_J$  and  $D_S$ ) minus a replacement index. From the equations above, the following relationships can easily be derived:

$$Rich_J = D_J - \beta_{-3} = \frac{\text{abs}(p_1 - p_2)}{p_1 + p_2 - p_1p_2}$$

$$Rich_S = D_S - Repl_S = \frac{\text{abs}(p_1 - p_2)}{p_1 + p_2}$$

$$\beta_{jne} = D_J - \beta_{jtu} = \frac{\max(p_1, p_2) \text{abs}(p_1 - p_2)}{2(p_1 + p_2) - 3p_1p_2 - \max(p_1^2, p_2^2)(1 - \min(p_1, p_2))} \quad (Nes_{BJ} \text{ in this Appendix})$$

$$\beta_{nes} = D_S - \beta_{sim} = \frac{\max(p_1, p_2) \text{abs}(p_1 - p_2)}{p_1 + p_2} \quad (Nes_{BS} \text{ in this Appendix})$$

These equations show that richness difference and nestedness are independent of the values of  $r_1$  and  $r_2$ . They depend only on  $p_1$  and  $p_2$ .

**7. Conclusion and summary**

This appendix attempted to describe in an orderly fashion the development of indices that decompose dissimilarity coefficients into replacement and richness/abundance difference (or nestedness) components. In the Podani and Baselga families, each one contains indices for presence-absence data that decompose the Jaccard and Sørensen dissimilarities, as well as indices

for species abundance data that decompose the Ružička and percentage difference dissimilarities. Both families were completed by new indices described in the present paper.

From the discussions that appeared in the recent literature, I chose to discuss the following points:

- As shown by Podani & Schmera (2011) and following papers, it is the numerators of the proposed indices that estimate replacement and richness difference. One can then scale the indices to values between 0 and 1 with denominators of one's choice, depending on the purpose of the study. The denominators of the Jaccard, Sørensen, Ružička and percentage difference dissimilarities, or those used by Baselga (2010, 2012) in his replacement (turnover) indices, can all be used. Ecologists should understand, however, that the chosen denominators may create distortions in the positioning of sites in an ordination, compared to using the numerator values only. None of the denominators proposed up to now have all the optimal qualities. The discussions about over- or under-estimation of species replacement by indices of the two families of indices are, actually, discussions about the choice of a denominator.
- The indices in the Podani family correspond to the concepts of replacement and richness/abundance difference. Those in the Baselga family are replacement (or turnover) and nestedness indices. Richness difference is not the same as nestedness. Podani & Schmera (2011) proposed an index of nestedness ( $N_{rel}$ ) that differs from their index of richness difference; they explained that the latter only represents a portion of nestedness; see the Introduction of the main paper. Hence the Baselga nestedness indices ( $Nes_{BJ}$  and  $Nes_{BS}$ ) should be compared to Podani & Schmera's relativized nestedness index, not to the richness difference indices of the Podani family ( $Rich_J$  and  $Rich_S$ ).
- In the two families, the replacement and richness difference (Podani family) or replacement and nestedness indices (Baselga family) sum to dissimilarity measures ( $D_J$ ,  $D_S$ ,  $D_R$ ,  $D_{\%diff}$ ) that are appropriate for beta diversity assessment, following the criteria of Legendre & De Cáceres (2013). An important point is that these indices are not themselves indices of beta diversity; they decompose dissimilarity coefficients that can be used as estimates of beta diversity.
- Replacement and richness difference or nestedness indices should have an ecological interpretation. In that respect, indices in the Podani family are easy to interpret due to the logic of their construction. Likewise, interpretation of Baselga's replacement indices is clear, whereas that of his nestedness indices is more intricate, albeit logical.
- When matrices of indices are to be used to produce ordinations of the sites, the Podani-family *RichDiff*/*AbDiff* indices ( $RichDiff_S$  and  $AbDiff_{\%diff}$ ) that decompose the Sørensen and percentage difference dissimilarities present clear advantages for ordination because the **RichDiff<sub>S</sub>** and **AbDiff<sub>%diff</sub>** matrices are Euclidean.
- Claims have been made that the *Repl* indices in the Podani family were correlated to species richness differences between the sampling units whereas indices in the Baselga family are not. Actually, all indices described in this appendix do not depend directly on site richness since they can all be expressed without recourse to the species richness of the sites that are compared,  $r_1$  and  $r_2$ . Section 6 of this appendix has shown that they can all be expressed by equations containing only  $p_1$  and  $p_2$ , where  $p_1$  is the proportion of shared species in the first sampling unit,  $p_1 = a/r_1$ , and  $p_2$  is the proportion of shared species in the second sampling unit,  $p_2 = a/r_2$ ;  $a$  is the number

of species in common between the two sites. So this criticism does not apply to any of the indices described in this appendix.

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Table S1.1. Measures of dissimilarity, replacement and richness difference for presence-absence data with names used by different authors. Modified and expanded from Carvalho *et al.* (2013).

Indices	Equation	Reference
<b>Dissimilarity indices</b>		
$D_J$ or $D_{\text{Jaccard}}$ or $\beta_{\text{CC}}$ or $\beta_{\text{jac}}$	$(b+c) / (a+b+c)$	Jaccard (1908)
$D_S$ or $D_{\text{Sørensen}}$ or $\beta_{\text{Sor}}$	$(b+c) / (2a+b+c)$	Sørensen (1948)
<b>Podani family, Jaccard</b>		
$\beta_{-3}$ or $R_{\text{rel}}$ or $\text{Repl}_J$	$\frac{2 \min(b,c)}{a + b + c}$	Williams (1996) Cardoso <i>et al.</i> (2009) Podani & Schmera (2011)
$\beta_{\text{rich}}$ or $D_{\text{rel}}$ or $\text{RichDiff}_J$	$\frac{ b - c }{a + b + c}$	Podani & Schmera (2011) Carvalho <i>et al.</i> (2012, 2013)
<b>Podani family, Sørensen</b>		
$\text{Repl}_S$	$\frac{2 \min(b,c)}{2a + b + c}$	Carvalho <i>et al.</i> (2013)
$\text{RichDiff}_S$	$\frac{ b - c }{2a + b + c}$	Carvalho <i>et al.</i> (2013)
<b>Baselga family, Jaccard</b>		
$\beta_{\text{Jtu}}(\text{Repl}_{BJ})$	$\frac{2 \min(b,c)}{a + 2 \min(b,c)}$	Baselga (2012)
$\beta_{\text{jne}}(\text{Nes}_{BJ})$	$D_J - \beta_{\text{Jtu}} = \frac{ b - c }{a + b + c} \times \frac{a}{a + 2 \min(b,c)}$	Baselga (2012)
<b>Baselga family, Sørensen</b>		
$\beta_{\text{sim}}(\text{Repl}_{BS})$	$\frac{2 \min(b,c)}{2a + 2 \min(b,c)} = \frac{\min(b,c)}{a + \min(b,c)}$	Lennon <i>et al.</i> (2001), Baselga (2010)
$\beta_{\text{nes}}(\text{Nes}_{BS})$	$D_S - \beta_{\text{sim}} = \frac{ b - c }{2a + b + c} \times \frac{a}{a + \min(b,c)}$	Baselga (2010)

Table S1.2. Podani-family indices: construction of the replacement (*Repl*), richness difference (or abundance difference for quantitative data) (*RichDiff* or *AbDiff*), and dissimilarity (*D*) indices, for presence-absence and abundance data. References for the indices, presence-absence data, Jaccard group: Podani & Schmera (2011); Sørensen group: Carvalho *et al.* (2013). Abundance indices, Jaccard group: Podani *et al.* (2013); Sørensen group: new in this paper.

	Presence-absence data	Species abundance data
<b>Numerators (num.)</b>		
Replacement num.	$2 \times \min(b, c) = (b + c) -  b - c $	$2 \times \min(B, C)$
Richness or abund. difference num.	$ b - c  = \max(b, c) - \min(b, c)$	$ B - C $
Dissimilarity num.	$(b + c) = 2 \times \min(b, c) +  b - c $	$(B + C) = 2 \times \min(B, C) +  B - C $
<b>Jaccard group (J)</b>		
Denominator	$(a + b + c)$	$(A + B + C)$
<i>D</i>	Jaccard dissimilarity: $D_J = (b + c) / (a + b + c)$	Ružička dissimilarity: $D_R = (B + C) / (A + B + C)$
<i>Repl</i>	$Repl_J = 2 \times \min(b, c) / (a + b + c)$	$Repl_R = 2 \times \min(B, C) / (A + B + C)$
<i>RichDiff/AbDiff</i>	$RichDiff_J =  b - c  / (a + b + c)$	$AbDiff_R =  B - C  / (A + B + C)$
<b>Sørensen group (S)</b>		
Denominator	$(2a + b + c)$	$(2A + B + C)$
<i>D</i>	Sørensen dissimilarity: $D_S = (b + c) / (2a + b + c)$	Percentage difference dissimilarity: $D_{\%diff} = (B + C) / (2A + B + C)$
<i>Repl</i>	$Repl_S = 2 \times \min(b, c) / (2a + b + c)$	$Repl_{\%diff} = 2 \times \min(B, C) / (2A + B + C)$
<i>RichDiff/AbDiff</i>	$RichDiff_S =  b - c  / (2a + b + c)$	$AbDiff_{\%diff} =  B - C  / (2A + B + C)$



Table S1.3. Baselga-family indices: construction of the replacement (*Repl*), nestedness (or abundance gradient component for quantitative data, *Nes*), and dissimilarity (*D*) indices, for presence-absence and abundance data. References for the indices, presence-absence data, Jaccard group: Baselga (2012); Sørensen group: Baselga (2010). Abundance indices, Jaccard group: new in this paper; Sørensen group: Baselga (2013).

	Presence-absence data	Species abundance data
<b>Jaccard group (<i>J</i>)</b>		
<i>D</i>	Jaccard dissimilarity: $D_J = (b+c) / (a+b+c)$	Ružička dissimilarity: $D_R = (B+C) / (A+B+C)$
<i>Repl</i>	$Repl_{BJ} = \frac{2\min(b,c)}{a + 2\min(b,c)}$	$Repl_{BR} = \frac{2\min(B,C)}{A + 2\min(B,C)}$
<i>Nes</i>	$Nes_{BJ} = \frac{ b-c }{a+b+c} \times \frac{a}{a + 2\min(b,c)}$	$Nes_{BR} = \frac{ B-C }{A+B+C} \times \frac{A}{A + 2\min(B,C)}$
<b>Sørensen group (<i>S</i>)</b>		
<i>D</i>	Sørensen dissimilarity: $D_S = (b+c) / (2a+b+c)$	Percentage difference dissimilarity: $D_{\%diff} = (B+C) / (2A+B+C)$
<i>Repl</i>	$Repl_{BS} = \frac{\min(b,c)}{a + \min(b,c)}$	$Repl_{B\%diff} = \frac{\min(B,C)}{A + \min(B,C)}$
<i>Nes</i>	$Nes_{BS} = \frac{ b-c }{2a+b+c} \times \frac{a}{a + \min(b,c)}$	$Nes_{B\%diff} = \frac{ B-C }{2A+B+C} \times \frac{A}{A + \min(B,C)}$

Table S1.4. Metric and Euclidean properties of the two families of indices: (a) Podani family, (b) Baselga family. Yes: the index has the property; No: the index does not have the property. Abbreviations:  $D$  = dissimilarity,  $Repl$  = replacement,  $RichDiff/AbDiff$  = richness/abundance difference,  $Nes$  = nestedness,  $J$  = Jaccard,  $R$  = Ružička,  $S$  = Sørensen,  $\%diff$  = percentage difference.

(a) Podani family	Metric property		Euclidean property	
	$index$	$\sqrt{index}$	$index$	$\sqrt{index}$
Jaccard group				
$D_J$	Yes	Yes	No	Yes
$D_R$	Yes	Yes	No	Yes
$Repl_J$	No	No	No	No
$Repl_R$	No	No	No	No
$RichDiff_J$	No	No	No	No
$AbDiff_R$	No	No	No	No
Sørensen group				
$D_S$	No	Yes	No	Yes
$D\%diff$	No	Yes	No	Yes
$Repl_S$	No	No	No	No
$Repl\%diff$	No	No	No	No
$RichDiff_S$	Yes	Yes	Yes	Yes
$AbDiff\%diff$	Yes	Yes	Yes	Yes
(b) Baselga family	Metric property		Euclidean property	
	$index$	$\sqrt{index}$	$index$	$\sqrt{index}$
Jaccard group				
$D_J$	Yes	Yes	No	Yes
$D_R$	Yes	Yes	No	Yes
$Repl_{BJ}$	No	No	No	No
$Repl_{BR}$	No	No	No	No
$Nes_{BJ}$	No	No	No	No
$Nes_{BR}$	No	No	No	No
Sørensen group				
$D_S$	No	Yes	No	Yes
$D\%diff$	No	Yes	No	Yes
$Repl_{BS}$	No	No	No	No
$Repl_B\%diff$	No	No	No	No
$Nes_{BS}$	No	No	No	No
$Nes_B\%diff$	No	No	No	No

*Appendix to:*

Legendre, P. Interpreting the replacement and richness difference components of beta diversity. *Global Ecology and Biogeography* (submitted).

## *Appendix S2*

### Simulations for monotonicity

Carvalho *et al.* (2013, pp. 830-831) carried out a simulation study to determine if the replacement and richness difference indices increased monotonically along ecological gradients showing increases in the amounts of replacement and richness difference.

- The replacement gradient was generated as follows: starting with a community containing  $p$  species ( $p = 105$  in our study), an increasing number of species were replaced at each time step during 25 steps. Each replacement involved one species that was present at time 1 and was lost at time 2, and one new species that appeared at time 2. At each time step, one more species was replaced than at the previous step.
- Three scenarios were used to simulate gradients of richness difference, with one, two, or three species lost at each step. In scenario 1, replacement dominates the gradient because two new species are involved in replacement at each step compared to one for richness difference. The two processes are of equal importance in scenario 2, and richness difference dominates in scenario 3.

There would, of course, be other ways of generating these gradients.

First, I reproduced the study made by these authors for the Podani & Schmera (2011) indices decomposing the Jaccard dissimilarity  $D_J$ . The results were similar to those obtained by Carvalho *et al.* (2013) (Fig. S2.1, upper row).

The study was repeated for the indices derived from the Sørensen dissimilarity  $D_S$ , which had not been considered by Carvalho *et al.* (2013) in their simulation study. The indices derived from  $D_S$  were monotonic to replacement and richness gradients (Fig. S2.1, lower row).

Next, I carried out simulations involving the relativized nestedness index of Podani & Schmera (2011) and Baselga's nestedness indices decomposing  $D_J$  and  $D_S$ . (Fig. S2.2). The results showed that the relativized nestedness index ( $N_{rel}$ ) decreased monotonically when replacement and richness difference increased (Fig. S2.2, upper row), whereas Baselga's nestedness-resultant  $D$  indices increased, then decreased (red lines in the middle and lower rows).

Finally, simulations were carried out to verify if the quantitative indices of the Podani-family obeyed the monotonicity condition of Carvalho *et al.* (2013).

- At each step in the simulations, which involved 100 species, selected species were replaced by new species, but without loss of total individuals, forming a gradient of increasing species replacement.
- Other species were lost, contributing to a smooth gradient of monotonic change in the abundance difference. The remaining initial species lost a constant number of individuals at each

step, following the *Ordered Comparison Case Series* simulation method proposed by Hajdu (1981) and used by Gower & Legendre (1986) to assess the properties of dissimilarity coefficients; these changes contributed to forming a smooth gradient of individual-based abundance differences along the series.

The *Repl* and *AbDiff* forms of the Ružička and percentage difference indices reacted monotonically to these quantitative changes in community composition (Fig. S2.3). The R code used to simulate the data is shown below. The indices were computed by function `beta.div.comp` (Appendix S3).

## References

- Carvalho, J.C., Cardoso, P., Borges, P.A.V., Schmera, D. & Podani, J. (2013) Measuring fractions of beta diversity and their relationships to nestedness: a theoretical and empirical comparison of novel approaches. *Oikos*, **122**, 825–834.
- Gower, J.C. & Legendre, P. (1986) Metric and Euclidean properties of dissimilarity coefficients. *Journal of Classification*, **3**, 5–48.
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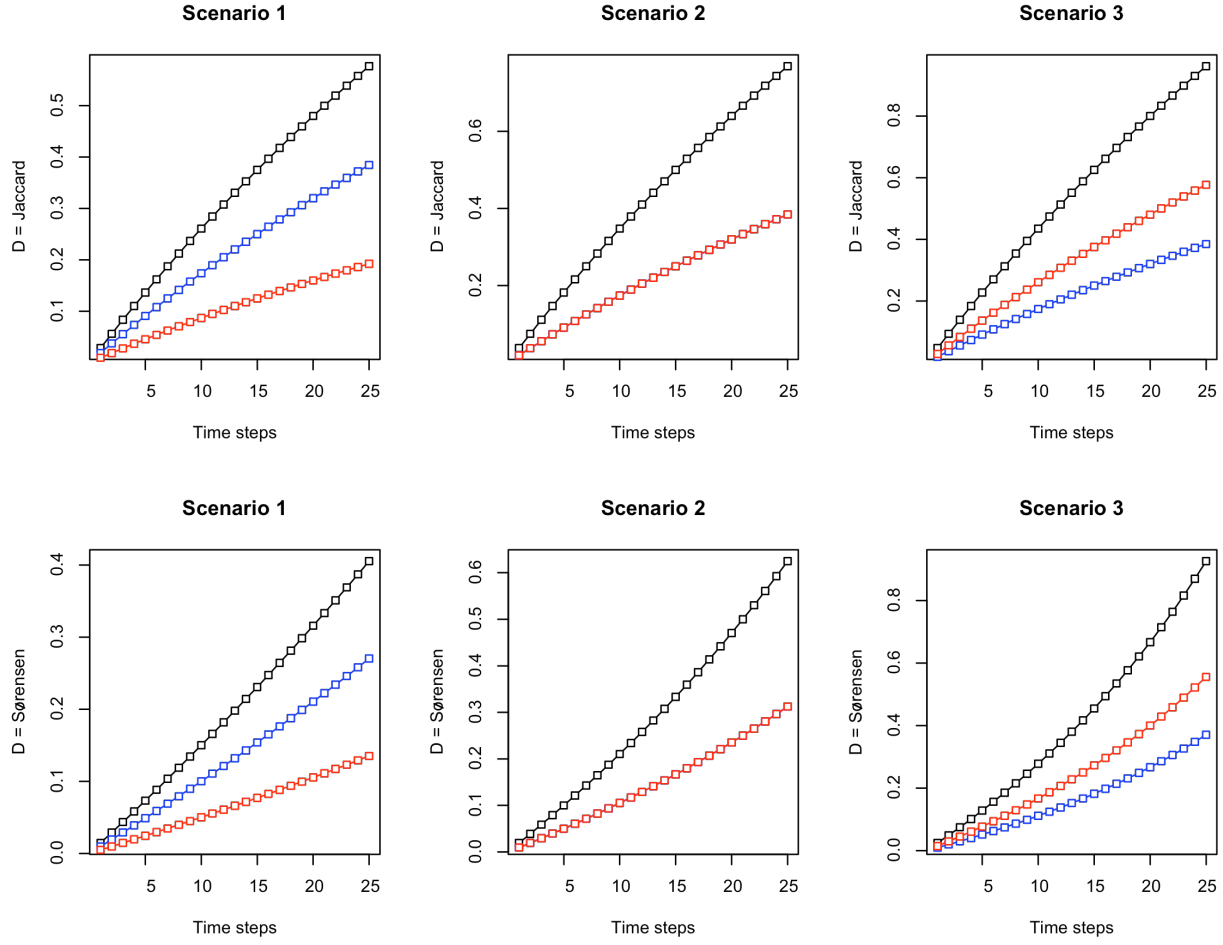


Figure S2.1 Simulation results for binary data. Podani & Schmera (2011) indices decomposing the Jaccard ( $D_J$ , upper row) and the Sørensen ( $D_S$ , lower row) dissimilarities. In each graph, the *initial* species data are compared to those at the given step along the simulated gradient (e.g. time). Black: dissimilarity values; blue: *Repl* index; red: *RichDiff* index. Under scenario 2, the *Repl* and *RichDiff* values are identical; the red squares are masking the blue symbols.

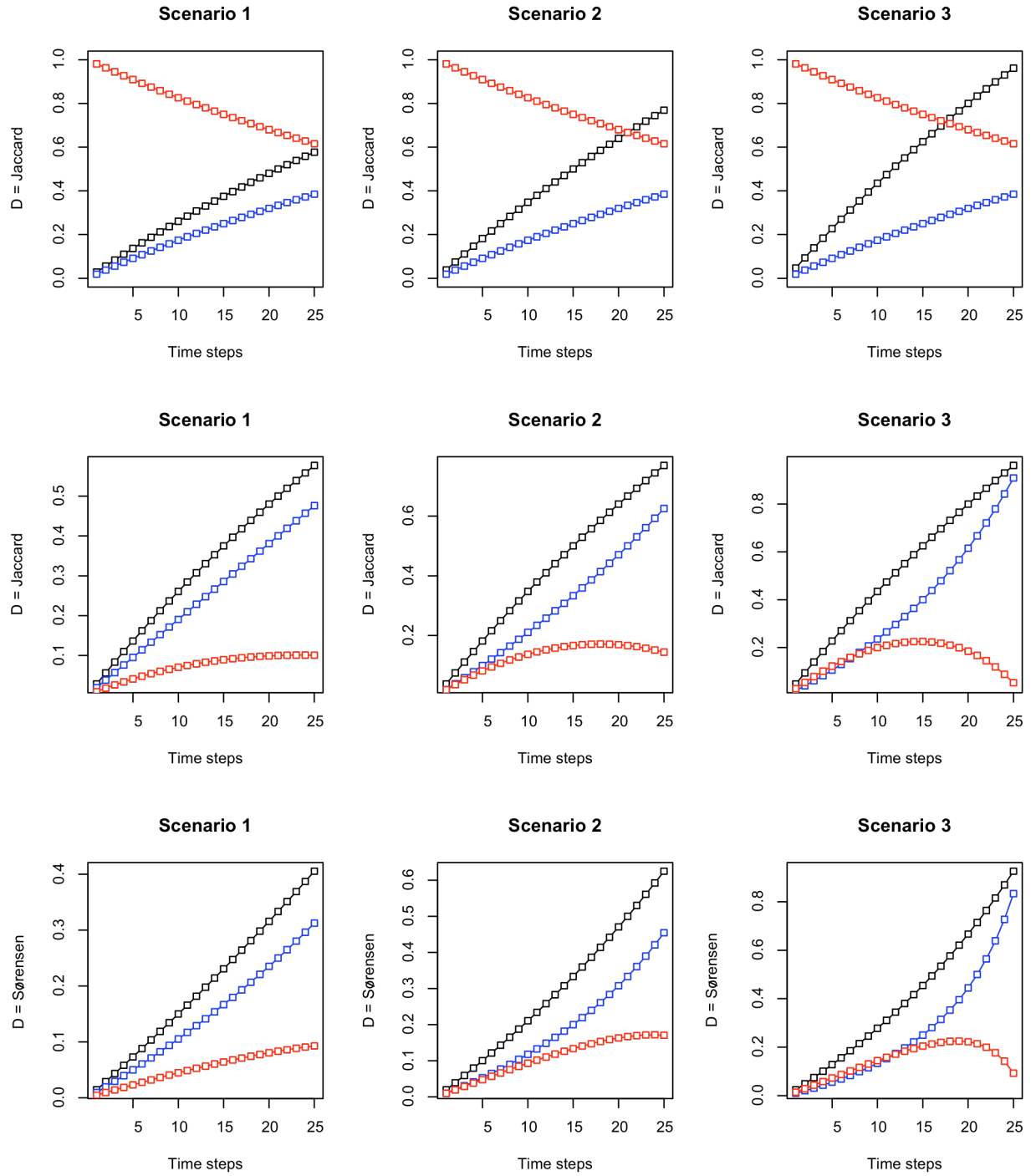


Figure S2.2 Simulation results for binary data. Upper row: Podani & Schmera (2011) decomposition of  $D_J$  into  $Repl$  and nestedness ( $N_{rel}$ ); middle row: Baselga-family decomposing  $D_J$ ; lower row: Baselga-family decomposing  $D_S$ . Black: dissimilarity values; blue:  $Repl$  indices; red:  $nestedness$  indices.

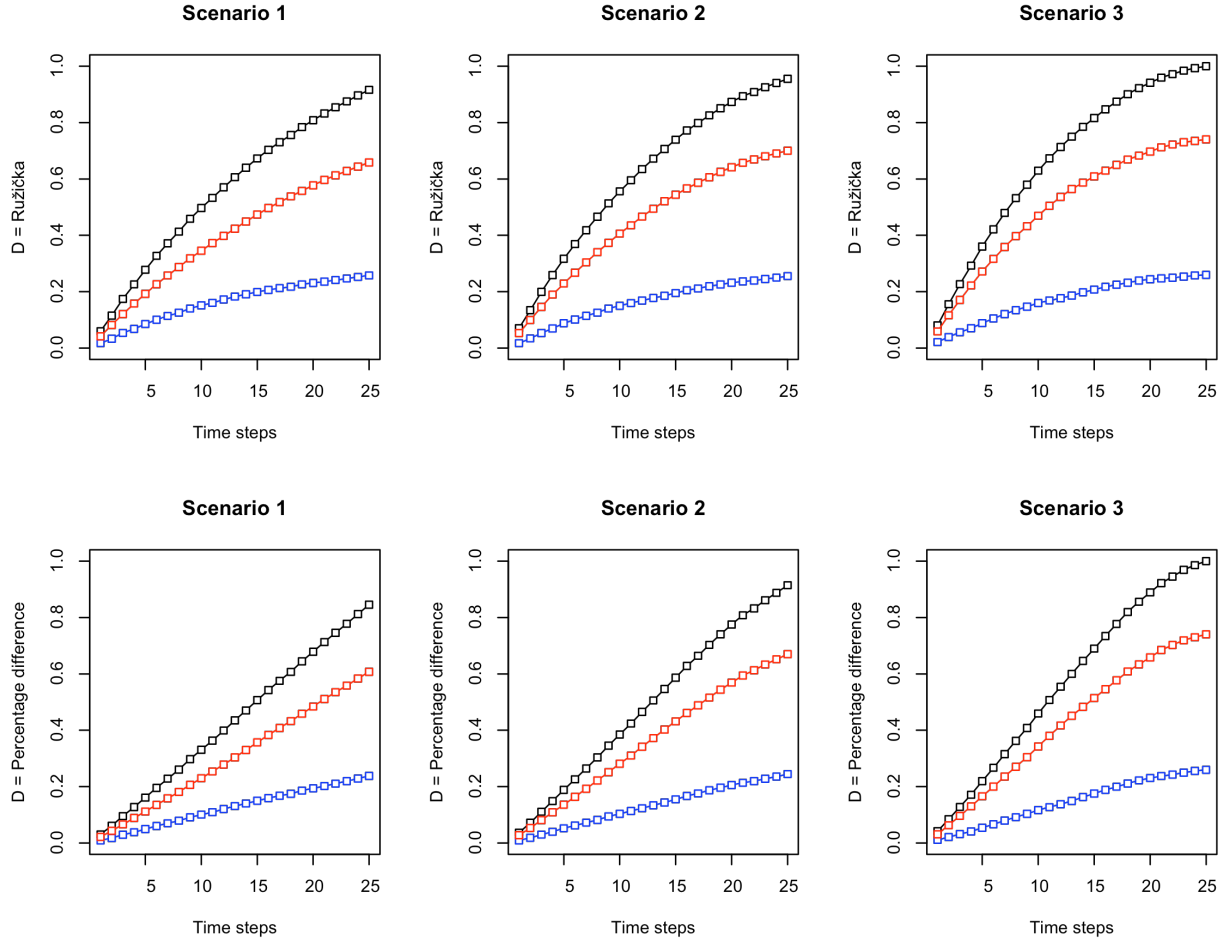


Figure S2.3 Simulation results for quantitative data. Podani-family indices decomposing the Ružička ( $D_R$ , upper row) and the percentage difference ( $D_{\%diff}$ , lower row) dissimilarities. In each graph, the initial species abundance data are compared to those at the given step along the simulated gradient (e.g. time). Black: dissimilarity values; blue: *Repl* index; red: *AbDiff* index.

## R functions that generated the simulated data

```

carvalho.simul <- function(steps=25, p.init=100, scenario=2, a.min=5, val=1)
#
# Simulations using species presence-absence data to determine if the
# replacement and richness difference indices respond monotonically to
# gradients. See Carvalho et al. (2013, pp. 830:831) for details.
#
# steps : Number of (temporal) simulation steps after the initial vector.
# p.init : Number of species present at reference site 1.
# scenario={1,2,3} : how many species are lost at each step.
#           =1 : lose one species at each step.
#           =2 : lose two species at each step.
#           =3 : lose three species at each step.
# a.min : Minimum number of species in common, in scenario #3, between the
#         initial data (data row 1) and the last time step (data row 26).
# val : constant species abundance, e.g. 1 (binary) or 10 (quantitative).
#
# License: GPL-2
# Author:: Pierre Legendre, August 2013
{
# Modify p.init to insure there are species in common (a.min > 0) between the
# initial and last time steps in scenario #3.
p.init <- p.init+a.min
# Simulated data matrix
mat = matrix(0,(steps+1),(p.init+steps))
#
p = p.init      # Initial no. of species for computation of richness difference
loss = 0
gain = 0
mat[1,1:p] = val
for(i in 2:(steps+1)) {
  loss = loss+scenario
  gain = gain+1
  p = p-1
  # cat("[",i,","],"p",p," loss",loss," gain",gain,"\n")
  #
  if((p-loss)>0) mat[i,(loss+1):p] = val
  mat[i,(p.init+1):(p.init+gain)] = val
}
mat
}

```



```

abundance.simul <- function(steps=25,p.init=100,scenario=2,val=10,cst.loss=1)
#
# Simulations using species abundance data to determine if the quantitative
# forms of the replacement and abundance difference indices respond
# monotonically to gradients. Method modified from that of Carvalho et al.
# (2013, pp. 830:831)
#
# Initial community: 'p.init' species, each with a runif() abundance.
# In the following (temporal) simulation steps:
#   Some species are lost (beginning of the vector).
#   Some species are replaced, with no loss of individuals.
#   The remaining initial species lose 1 individual each step (as in OCCAS).
#
# steps : Number of (temporal) simulation steps after the initial vector.
# p.init : Number of species present at reference site 1.
# scenario={1,2,3} : how many species are lost at each step.
#   =1 : lose one species at each step.
#   =2 : lose two species at each step.
#   =3 : lose three species at each step.
# val : Upper bound of values generated by runif().
# cst.loss : constant loss at each step for the initial species.
#
# License: GPL-2
# Author:: Pierre Legendre, August 2013
{
mat = matrix(0,(steps+1),(p.init+steps))
#
p = p.init      # number of non-zero data in initial species vector
loss = 0
gain = 0
mat[1,1:p] = floor(runif(p,1,(val+1)))+cst.loss*steps
#
for(i in 2:(steps+1)) {
# Beginning of vector 1:((i-1)*scenario): lost sp. (measured by RichDiff, red)
# Losses associated with replacements: (p.init-(i-2)): p.init)
# Gains associated with replacements: (p.init+1): (p.init+(i-1)) (Repl, blue)
# => Maintain the number of individuals constant through all steps
  loss = loss+scenario
  gain = gain+1
  p = p-1
  # cat("[",i,",","]","p",p," loss",loss," gain",gain,"\n")
  if((p-loss)>0) mat[i,(loss+1):p] = mat[(i-1),(loss+1):p]-cst.loss
  #
  lost.ind.repl <- sum(mat[(i-1),(p.init-(i-2)):p.init])
  n.per.new <- lost.ind.repl/gain
  # cat("lost.ind.repl =",lost.ind.repl," gain =",gain," n.per.new
=" ,n.per.new,"\n")
  mat[i,(p.init+gain)] = n.per.new # Abundance of the (one) new species
  if(i>2) mat[i,(p.init+1):(p.init+(gain-1))]
    = mat[(i-1),(p.init+1):(p.init+(gain-1))]+n.per.new
}
mat
}

```

```
# Appendix to:

# Legendre, P. Interpreting the replacement and richness difference components
# of beta diversity. Global Ecology and Biogeography (submitted).

#                                     Appendix S3
#
# R function to compute the Podani- and Baselga-family decompositions of the
# Jaccard or Sørensen groups into replacement and richness/abundance difference
# (or nestedness) components, for species presence-absence or abundance data.

beta.div.comp <- function(mat, coef="J", quant=FALSE, save.abc=FALSE)
#
# Description --
#
# Podani-family and Baselga-family decompositions of the Jaccard and Sørensen
# dissimilarity coefficients into replacement and richness/abundance difference
# components, for species presence-absence or abundance data, as described
# in Legendre (submitted).
#
# Usage --
#
# beta.div.comp(mat, coef="J", quant=FALSE, save.abc=FALSE)
#
# Arguments --
#
# mat : Data in matrix or data.frame form.
# coef : Family of coefficients to be computed --
#       "S" or "Sorensen": Podani family, Sørensen-based indices
#       "J" or "Jaccard" : Podani family, Jaccard-based indices
#       "BS" : Baselga family, Sørensen-based indices
#       "BJ" : Baselga family, Sørensen-based indices
#       "N" : Podani & Schmera (2011) relativized nestedness index.
#       The quantitative form in Sørensen family is the percentage difference.
#       The quantitative form in the Jaccard family is the Ruzicka index.
#
# quant=TRUE : Compute the quantitative form of the indices and D.
#             =FALSE: Compute the presence-absence form of the coefficients.
# save.abc=TRUE : Save the matrices of parameters a, b and c used in the
#                 presence-absence calculations.
#
# Details --
#
# For species presence-absence data, the distance coefficients are
# Jaccard=(b+c)/(a+b+c) and Sørensen=(b+c)/(2*a+b+c) with usual abc notation.
#
# For species abundance data, the distance coefficients are
# the Ruzicka index = (B+C)/(A+B+C) and Odum's percentage difference
# (incorrectly called Bray-Curtis) = (B+C)/(2A+B+C), where
# A = sum of the intersections (or minima) of species abundances at two sites,
# B = sum at site 1 minus A, C = sum at site 2 minus A.
#
# The binary (quant=FALSE) and quantitative (quant=TRUE) forms of the S and
# J indices return the same values when computed for presence-absence data.
#
```

---

```
# Value --
#
# repl : Replacement matrix, class = 'dist'.
# rich : Richness/abundance difference or nestedness matrix, class = 'dist'.
#       With options "BJ", "BS" and "N", 'rich' contains nestedness indices.
#       With option "N", the 'repl' and 'rich' values do not add up to 'D'.
# D     : Dissimilarity matrix, class = 'dist'.
# part  : Beta diversity partitioning --
#       1. Total beta div. = sum(D.ij)/(n*(n-1)) (Legendre & De Cáceres 2013)
#       2. Total replacement diversity
#       3. Total richness/abundance difference diversity (or nestedness)
#       4. Total replacement div./Total beta div.
#       5. Total richness/abundance diff. div. (or nestedness)/Total beta div.
# Note  : Name of the dissimilarity coefficient.
#
# References --
#
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# diversity. Global Ecology and Biogeography, 19, 134–143.
#
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#
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#
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#
# Podani, J. & Schmera, D. 2011. A new conceptual and methodological framework
# for exploring and explaining pattern in presence-absence data. Oikos, 120,
# 1625–1638.
#
# License: GPL-2
# Author:: Pierre Legendre
{
coef <- pmatch(coef, c("S", "J", "BS", "BJ", "N"))
if(coef==5 & quant) stop("coef='N' and quant=TRUE: combination not programmed")
mat <- as.matrix(mat)
n <- nrow(mat)
if(is.null(rownames(mat))) noms <- paste("Site",1:n,sep="")
  else noms <- rownames(mat)
#
if(!quant) {      # Binary data provided, or make the data binary
  if(coef==1) form="Podani family, Sorensen"
  if(coef==2) form="Podani family, Jaccard"
```

```
if(coef==3) form="Baselga family, Sorensen"
if(coef==4) form="Baselga family, Jaccard"
if(coef==5) form="Podani & Schmera (2011) relativized nestedness"
mat.b <- ifelse(mat>0, 1, 0)
a <- mat.b %*% t(mat.b)
b <- mat.b %*% (1 - t(mat.b))
c <- (1 - mat.b) %*% t(mat.b)
min.bc <- pmin(b,c)
#
if(coef==1 || coef==2) {
  repl <- 2*min.bc # replacement, turnover, beta-3
  rich <- abs(b-c) # nestedness, richness diff., beta-rich
  #
  # Add the denominators
  if(coef==1) { # Sørensen-based components
    repl <- repl/(2*a+b+c)
    rich <- rich/(2*a+b+c)
    D <- (b+c)/(2*a+b+c)
  } else if(coef==2) { # Jaccard-based components
    repl <- repl/(a+b+c)
    rich <- rich/(a+b+c)
    D <- (b+c)/(a+b+c)
  }
} else if(coef==3) { # Baselga 2010 components based on Sørensen
  D <- (b+c)/(2*a+b+c) # Sørensen dissimilarity
  repl <- min.bc/(a+min.bc) # replacement, turnover
  rich <- D-repl # nestedness-resultant dissimilarity
} else if(coef==4) { # Baselga 2012 components based on Jaccard
  D <- (b+c)/(a+b+c) # Jaccard dissimilarity
  repl <- 2*min.bc/(a+2*min.bc) # replacement, turnover
  rich <- D-repl # nestedness-resultant dissimilarity
} else if(coef==5) { # rich = Podani N = nestedness based on Jaccard
  repl <- 2*min.bc/(a+b+c)
  D <- (b+c)/(a+b+c)
  rich <- matrix(0,n,n)
  for(i in 2:n) {
    for(j in 1:(i-1)) {
      aa = a[i,j]; bb = b[i,j]; cc = c[i,j]
      if(a[i,j] == 0) rich[i,j] <- 0
      else rich[i,j] <- (aa + abs(bb-cc))/(aa+bb+cc)
    }
  }
}

rownames(repl) <- rownames(rich) <- rownames(D) <- noms
D <- as.dist(D)
repl <- as.dist(repl)
rich <- as.dist(rich)
total.div <- sum(D)/(n*(n-1))
repl.div <- sum(repl)/(n*(n-1))
rich.div <- sum(rich)/(n*(n-1))
part <- c(total.div,repl.div,rich.div,repl.div/total.div,rich.div/total.div)
#
if(save.abc) {
  res <- list(repl=repl, rich=rich, D=D, part=part, Note=form,
    a=as.dist(a), b=as.dist(b), c=as.dist(c))
}
```

---

```

    } else {
      res <- list(repl=repl, rich=rich, D=D, part=part, Note=form)
    }
#
} else {      # Quantitative data
# Calculations based on individuals.within.species
  if(coef==1) form<-"Podani family, percentage difference"
  if(coef==2) form<-"Podani family, Ruzicka"
  if(coef==3) form<-"Baselga family, percentage difference"
  if(coef==4) form<-"Baselga family, Ruzicka"
  # Baselga (2013) notation:
  # A = W = sum of minima in among-site comparisons
  # B = site.1 sum - W = K.1 - W
  # C = site.2 sum - W = K.2 - W
  K <- vector("numeric", n) # site (row) sums
  W <- matrix(0,n,n)
  repl <- matrix(0,n,n)
  rich <- matrix(0,n,n)
  D <- matrix(0,n,n)
  rownames(repl) <- rownames(rich) <- rownames(D) <- noms
  K <- apply(mat,1,sum) # Row sums
  for(i in 2:n) for(j in 1:(i-1)) W[i,j] <- sum(pmin(mat[i,], mat[j,]))
  #
  # Quantitative extensions of the S and J decompositions
  for(i in 2:n) {
    for(j in 1:(i-1)) {
      repl[i,j] <- 2*(min(K[i],K[j])-W[i,j]) # 2*min(B,C)
      rich[i,j] <- abs(K[i]-K[j]) # abs(B-C)
    }
  }
  #
  # Add the denominators
  if(coef==1) { # Sørensen-based (% difference) components
    for(i in 2:n) {
      for(j in 1:(i-1)) { # Baselga 2013 notation:
        repl[i,j] <- repl[i,j]/(K[i]+K[j]) # 2min(B,C)/(2A+B+C)
        rich[i,j] <- rich[i,j]/(K[i]+K[j]) # abs(B-C)/(2A+B+C)
        # cat(K[i], K[j], W[i,j],"\n")
        D[i,j] <- (K[i]+K[j]-2*W[i,j])/(K[i]+K[j]) # (B+C)/(2A+B+C)
      }
    }
  } else if(coef==2) { # Jaccard-based (Ruzicka) components
    for(i in 2:n) {
      for(j in 1:(i-1)) { # Baselga 2013 notation:
        repl[i,j] <- repl[i,j]/(K[i]+K[j]-W[i,j]) # 2min(B,C)/(A+B+C)
        rich[i,j] <- rich[i,j]/(K[i]+K[j]-W[i,j]) # abs(B-C)/(A+B+C)
        # cat(K[i], K[j], W[i,j],"\n")
        D[i,j] <- (K[i]+K[j]-2*W[i,j])/(K[i]+K[j]-W[i,j]) # (B+C)/(A+B+C)
      }
    }
  }
  #
  # Baselga (2013): quantitative extensions of the Baselga (2010) indices
  if(coef==3) { # Baselga (2013) indices decomposing percentage difference
    for(i in 2:n) {
      for(j in 1:(i-1)) {
        repl[i,j] <- (min(K[i],K[j])-W[i,j])/min(K[i],K[j])

```

```
rich[i,j] <- abs(K[i]-K[j])*W[i,j]/((K[i]+K[j])*min(K[i],K[j]))
# cat(K[i], K[j], W[i,j],"\n")
D[i,j] <- (K[i]+K[j]-2*W[i,j])/(K[i]+K[j])
}
}
}
if(coef==4) { # Decomposing Ruzicka in the spirit of Baselga 2013
  for(i in 2:n) {
    for(j in 1:(i-1)) {
      repl[i,j] <-
        2*(min(K[i],K[j])-W[i,j])/(2*min(K[i],K[j])-W[i,j])
      rich[i,j] <- abs(K[i]-K[j])*W[i,j]/
        ((K[i]+K[j]-W[i,j])*(2*min(K[i],K[j])-W[i,j]))
      # cat(K[i], K[j], W[i,j],"\n")
      D[i,j] <- (K[i]+K[j]-2*W[i,j])/(K[i]+K[j]-W[i,j])
    }
  }
}
#
repl <- as.dist(repl)
rich <- as.dist(rich)
D <- as.dist(D)
repl.div <- sum(repl)/(n*(n-1))
rich.div <- sum(rich)/(n*(n-1))
total.div <- sum(D)/(n*(n-1))
part <- c(total.div,repl.div,rich.div,repl.div/total.div,rich.div/total.div)
#
res <- list(repl=repl, rich=rich, D=D, part=part, Note=form)
}
res
}
```

# Appendix to:

# Legendre, P. Interpreting the replacement and richness difference components  
# of beta diversity. Global Ecology and Biogeography (submitted).

# Appendix S4

# R function to compute the dbRDA F-test of significance between response data  
# represented by a Euclidean or non-Euclidean dissimilarity matrix and a matrix  
# of explanatory variables, following McArdle and Anderson (2001).

```
dbRDA.D <- function(D, X, nperm=999, option=3, compute.eig=FALSE, coord=FALSE,  
rda.coord=2, positive.RDA.values=FALSE)
```

#  
# Description --

# Compute the dbRDA F-test of significance between response data represented by  
# a Euclidean or non-Euclidean dissimilarity matrix and a matrix of explanatory  
# variables, using the method of McArdle and Anderson (2001).

# Usage --

```
# dbRDA.D(D, X, nperm=999, option=3, compute.eig=FALSE, coord=FALSE,  
#         rda.coord=2, positive.RDA.values=FALSE)
```

# Arguments --

# D : Distance matrix representing the response data. D may be non-Euclidean.  
# X : Matrix of explanatory variables for the RDA, class 'data.frame' or  
# 'matrix'. Factors must be recoded as dummy variables or Helmert contrasts.  
# nperm : Number of permutations for the test of significance.

# option=1 : Original McArdle-Anderson (2001) equation 4. Slow, not recommended.  
# option=2 : McArdle-Anderson equation, simplified.  
# option=3 : Least-squares after orthogonalizing X.  
# SSY = sum(diag(G)), where G is the Gower-centred distance matrix,  
# SSYhat = sum(diag(H %\*% G %\*% H)), where H is the projector matrix.

# Option=1 -- The original F statistic of McArdle and Anderson (2001), eq. 4:  
#  $F = \text{SSYhat} / \text{sum}(\text{diag}(\text{I.minus.H} \%* \% G \%* \% \text{I.minus.H}))$   
# Degrees of freedom are added to this equation in the output list.  
# Option=2 -- Simplified equation:  
#  $F = \text{SSYhat} / (\text{SSY} - \text{SSYhat})$   
# Option=3 -- Orthogonalize matrix X by PCA before computing H. No inversion.  
# Compute SSYhat as above, then  $F = \text{SSYhat} / (\text{SSY} - \text{SSYhat})$   
# Opt. 2 and 3 are equivalent; they require half the computing time of option 1.

# compute.eig=TRUE : the eigenvalues and eigenvectors of D are computed.  
# => Do NOT use with very large matrices (slow).  
# coord=TRUE : compute the principal coordinates corresponding to the  
# positive eigenvalues of D. Requires that compute.eig=TRUE.  
# rda.coord : Number of RDA ordination coordinates to compute, for example 2.  
# positive.RDA.values=TRUE : store only positive RDA eigenvalues in output list.  
# =FALSE: store all RDA eigenvalues in output list.

# Details --

---

```
#
# Compute the dbRDA F-test of significance. The response is represented by a
# Euclidean or non-Euclidean dissimilarity matrix; X is a matrix of explanatory
# variables, as in regular RDA.
#
# The F-statistic is obtained without prior computation of the eigenvalues and
# eigenvectors of the dissimilarity matrix, hence no correction has to be made
# to eliminate the negative eigenvalues. Three computation methods are
# available, all derived from McArdle and Anderson (2001).
#
# The eigenvalues and eigenvectors of D are computed if compute.eig=TRUE.
# If coord=TRUE, the principal coordinates corresponding to the positive
# eigenvalues of D are computed.
#
# The function may fail to produce a meaningful RDA test of significance and
# ordination axes if D is extremely non-Euclidean. This is the case with some
# forms of genomic distances.
#
# Value --
#
# F : F-statistic.
# Rsquare : R-square and adjusted R-square statistics.
# P.perm : Permutational p-value of RDA R-square (test based on F).
# SS.total : Trace of matrix G, equal to the total sum of squares of Y and the
#             sum of the eigenvalues of D.
# PCoA.values : Eigenvalues (if they are computed, i.e. if compute.eig=TRUE).
# PCoA.vectors : Principal coordinates for the positive eigenvalues of D.
# RDA.values : RDA eigenvalues.
# RDA.rel.values : RDA relative eigenvalues.
# RDA.cum.values : RDA cumulative relative eigenvalues.
# RDA.coord : Ordination coordinates of objects on selected RDA axes.
#
# References --
#
# Legendre, P. and L. Legendre. 2012. Numerical ecology, 3rd English edition.
# Elsevier Science BV, Amsterdam.
#
# McArdle, B. H. and M. J. Anderson. 2001. Fitting multivariate models to
# community data: a comment on distance-based redundancy analysis.
# Ecology 82: 290-297.
#
# Example -- Six sites from the mite data available in the vegan package.
#
# library(vegan)
# Load function dbRDA.D()
# data(mite)
# data(mite.env)
# sel = c(14,24,31,41,49,64)
# mite.BC = vegdist(mite[sel,], "bray") # Two negative eigenvalues
# res = dbRDA.D(mite.BC, mite.env[sel,1:2], nperm=999, compute.eig=TRUE)
# plot(res$RDA.coord)
# text(res$RDA.coord, labels=rownames(mite.env[sel6,]), pos=3)
#
# License: GPL-2
# Author:: Pierre Legendre, March 2013
{
  D <- as.matrix(D)
```



```
X <- as.matrix(X)
n <- nrow(D)
epsilon <- .Machine$double.eps
#
# Gower centring, matrix formula. Legendre & Legendre (2012), equation 9.42
One <- matrix(1,n,n)
mat <- diag(n) - One/n
G <- -0.5 * mat %*% (D^2) %*% mat
SSY <- sum(diag(G))
# LCBD <- diag(G)
#
# Principal coordinate analysis after eigenvalue decomposition of D
if(compute.eig) {
  eig <- eigen(G, symmetric=TRUE)
  values <- eig$values      # All eigenvalues
  vectors <- eig$vectors    # All eigenvectors, scaled to lengths 1
  if(coord) {
    select <- which(values > epsilon)
    princ.coord <- vectors[,select] %*% diag(sqrt(values[select]))
  } else { princ.coord <- NA }
} else {
  values <- princ.coord <- NA
}
#
# Compute projector matrix H ("hat" matrix in the statistical literature)
X.c <- scale(X, center=TRUE, scale=FALSE) # Centre matrix X
m <- qr(X.c, tol=1e-6)$rank               # m = rank of X.c
cat("Rank of X centred =",m,"\n")
if(m==1) {
  H <- (X.c[,1] %*% t(X.c[,1]))/((t(X.c[,1]) %*% X.c[,1])[1,1])
} else {
  if(option<3) {
    # if(det(t(X.c)%*%X.c)<epsilon) stop ('Collinearity detected in X')
    if(m < ncol(X.c)) stop ('Collinearity detected in X')
    H <- X.c %*% solve(t(X.c) %*% X.c) %*% t(X.c)
    #
    # option=3: compute projector H from orthogonalized X; no inversion
  } else {
    X.eig <- eigen(cov(X.c))
    k <- length(which(X.eig$values > epsilon))
    X.ortho <- X.c %*% X.eig$vectors[,1:k] # F matrix of PCA
    XprX <- t(X.ortho) %*% X.ortho
    H <- X.ortho %*% diag(diag(XprX)^(-1)) %*% t(X.ortho)
  }
}
#
# Compute the F statistic: McArdle & Anderson (2001), equation 4 modified
HGH <- H %*% G %*% H
SSYhat <- sum(diag(HGH))
#
if(option==1) {
  I.minus.H <- diag(n) - H
  den1 <- sum(diag(I.minus.H %*% G %*% I.minus.H))
  F <- SSYhat/den1      # F statistic without the degrees of freedom
  Rsquare <- F/(F+1)
} else {
  F <- SSYhat/(SSY-SSYhat) # F statistic without the degrees of freedom
```

---

```
Rsquare <- SSYhat/SSY      # or equivalent: Rsquare <- F/(F+1)
}
RsqAdj <- 1-((1-Rsquare)*(n-1)/(n-1-m))
#
# Permutation test of F
if(nperm > 0) {
  nGE=1
  for(i in 1:nperm) {
    order <- sample(n)
    Gperm <- G[order, order]
    H.Gperm.H <- H %*% Gperm %*% H
    SSYhat.perm <- sum(diag(H.Gperm.H))
    #
    if(option==1) {
      den <- sum(diag(I.minus.H %*% Gperm %*% I.minus.H))
      F.perm <- SSYhat.perm/den
    } else {
      F.perm <- SSYhat.perm/(SSY-SSYhat.perm)
    }
    if(F.perm >= F) nGE=nGE+1
  }
  P.perm <- nGE/(nperm+1)
} else { P.perm <- NA }
#
# Compute RDA ordination coordinates
if(rda.coord > 0) {
  HGH.eig <- eigen(HGH, symmetric=TRUE)
  # kk <- length(which(HGH.eig$values > epsilon))
  RDA.values <- HGH.eig$values
  rel.eig <- RDA.values/SSY
  cum.eig <- cumsum(rel.eig)
  kk <- length(which(rel.eig > epsilon))
  if(positive.RDA.values) {
    RDA.values <- RDA.values[1:kk]
    rel.eig <- rel.eig[1:kk]
    cum.eig <- cum.eig[1:kk]
  }
  k <- min(rda.coord, kk)
  if(k >= 2) {
    RDA.coord <-sweep(HGH.eig$vectors[,1:k],2,sqrt(RDA.values[1:k]),FUN="*")
  } else {
    RDA.coord <- NA
    cat("k =",k," -- Fewer than two RDA eigenvalues > 0\n")
  }
} else { RDA.values <- rel.eig <- cum.eig <- RDA.coord <- NA }
#
list(F=F*(n-m-1)/m, Rsquare=c(Rsquare,RsqAdj), P.perm=P.perm, SS.total=SSY,
PCoA.values=values, PCoA.vectors=princ.coord, RDA.values=RDA.values/(n-1),
RDA.rel.values=rel.eig, RDA.cum.values=cum.eig, RDA.coord=RDA.coord)
}
```

```
# Appendix to:  
# Legendre, P. Interpreting the replacement and richness difference components  
# of beta diversity. Global Ecology and Biogeography (submitted).
```

```
#  
# Appendix S5
```

```
# R function to compute LCBd indices from a dissimilarity matrix (D) or from  
# beta diversity component matrices (Repl, RichDiff/AbDiff or Nes).
```

```
LCBD.comp <- function(x, sqrt.x=TRUE)
```

```
#  
# Description --  
#
```

```
# Computes LCBd indices (Legendre and De Cáceres 2013) from a dissimilarity  
# matrix (D) or beta div. component matrices (Repl, RichDiff/AbDiff or Nes).
```

```
#  
# Arguments --  
#
```

```
# x : D or beta diversity component matrix, class=dist.
```

```
# sqrt.x : Take sqrt() of components before computing LCBd.comp. Use
```

```
# sqrt.x=TRUE for the replacement and richness/abundance difference indices  
# computed by beta.div.comp(), as well as for the corresponding D matrices.
```

```
#  
# Reference --  
#
```

```
# Legendre, P. and M. De Cáceres. 2013. Beta diversity as the variance of  
# community data: dissimilarity coefficients and partitioning. Ecology  
# Letters 16: 951-963.
```

```
#  
# License: GPL-2  
# Author:: Pierre Legendre, August 2013
```

```
{  
### Internal function  
centre <- function(D,n)  
  # Centre a square matrix D by matrix algebra  
  # mat.cen = (I - 11'/n) D (I - 11'/n)  
  { One <- matrix(1,n,n)  
    mat <- diag(n) - One/n  
    mat.cen <- mat %*% D %*% mat  
  }  
}
```

```
###  
n <- nrow(as.matrix(x))
```

```
if(sqrt.x) {  
  # x = sqrt(x)  
  SStotal <- sum(x)/n # eq. 8  
  BDtotal <- SStotal/(n-1) # eq. 3  
  G <- centre(as.matrix(-0.5*x), n) # Gower-centred matrix  
} else {  
  SStotal <- sum(x^2)/n # eq. 8  
  BDtotal <- SStotal/(n-1) # eq. 3  
  G <- centre(as.matrix(-0.5*x^2), n) # Gower-centred matrix  
}
```

```
LCBD <- diag(G)/SStotal # Legendre & De Cáceres (2013), eq. 10b
```

```
out <- list(SStotal_BDtotal=c(SStotal,BDtotal), LCBd=LCBD, D=x)
```

```
}
```

Appendix to:

Legendre, P. Interpreting the replacement and richness difference components of beta diversity. *Global Ecology and Biogeography* (submitted).

## Appendix S6

### Principal coordinate ordinations

Principal coordinate (PCoA) ordinations of the Podani-family replacement and richness difference indices based on the Jaccard (Fig. S6.1) and Sørensen (Fig. S6.2) dissimilarities for the case study data. Detailed properties of these ordinations will be investigated in another study.

The ordinations in Fig. S6.1 are based upon replacement (**Repl<sub>J</sub>**) and richness difference (**RichDiff<sub>J</sub>**) matrices that are not Euclidean. Ordinations along the first principal coordinates are Euclidean but, as in all multivariate ordinations, the distances among sampling units are approximate. The ordination of the *RichDiff<sub>J</sub>* indices in Fig. S6.1b shows a less precise ordering of the sampling units than Fig. S6.2b, which is based upon the *RichDiff<sub>S</sub>* indices.

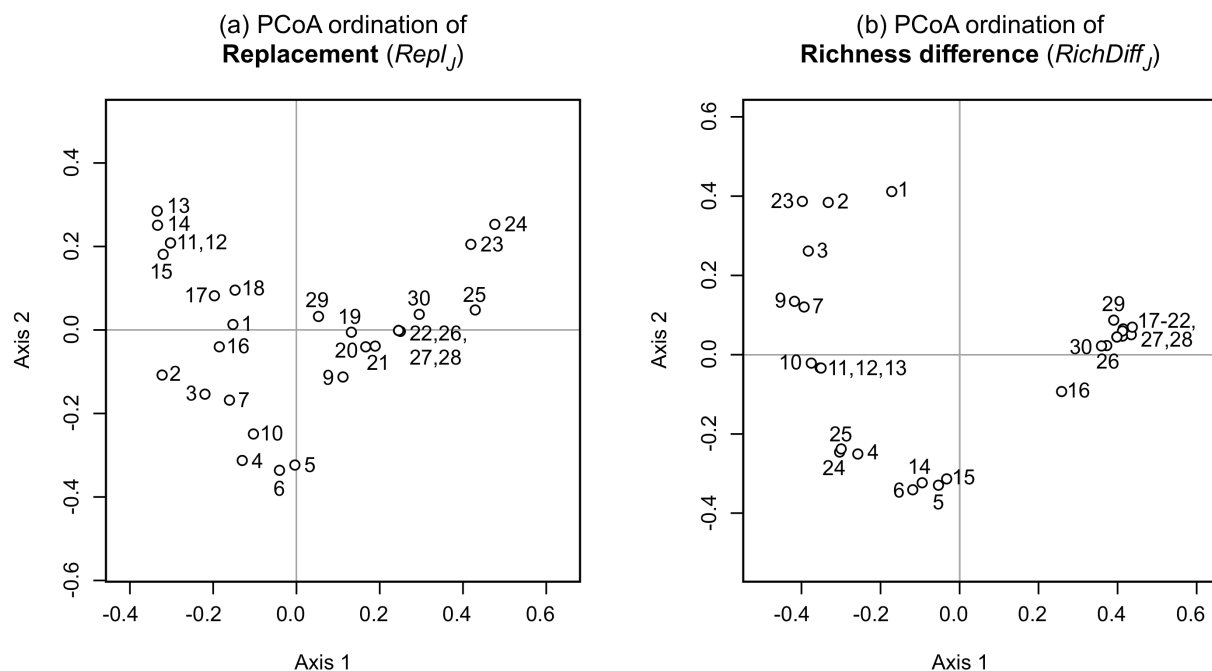


Figure S6.1 Principal coordinate ordinations of the Podani-family replacement and richness difference indices based on Jaccard dissimilarity for the fish case study data. PCoA of square-root transformed (a) replacement (*Repl<sub>J</sub>*) and (b) richness difference (*RichDiff<sub>J</sub>*) indices. These matrices are not Euclidean even after square-root transformation.

Of the four indices for species presence-absence data represented by ordinations in this appendix, the **RichDiff<sub>S</sub>** matrix is the only one that has the mathematical property of being Euclidean (Appendix S1, Table S1.4). The ordination in two dimensions (Fig. S6.2b) displays a precise ordering of the sampling units along the richness gradient, along which the sites form a curved one-dimensional ordination (i.e. a curved line). Site 1 (left of the graph) has the lowest richness with only 1 species whereas site 29 (right) is the richest with 26 species; 27 species were captured along the river. Sites 23-25 had reduced richness due to agricultural pollution; this caused reversal of the ordering of the sites by richness, compared to their geographical sequence.

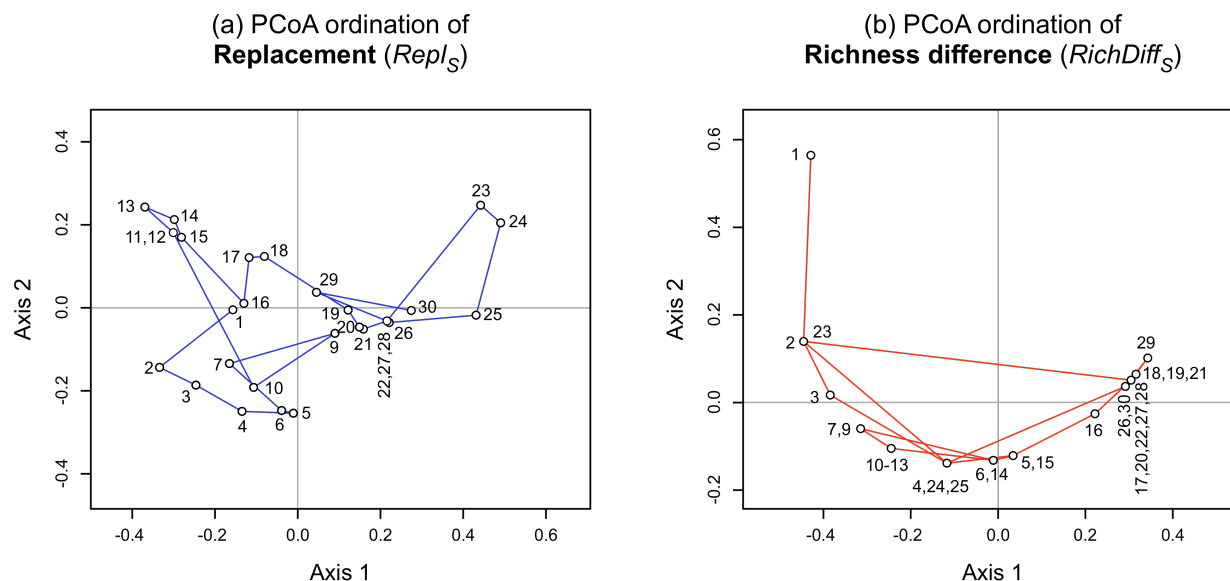


Figure S6.2 Principal coordinate ordinations of the Podani-family replacement and richness difference indices based on the Sørensen dissimilarity for the fish case study data. (a) PCoA of square-rooted replacement (*Repl<sub>S</sub>*) and (b) of untransformed richness difference (*RichDiff<sub>S</sub>*) indices. The **Repl<sub>S</sub>** matrix is not Euclidean even after square-root transformation whereas the **RichDiff<sub>S</sub>** matrix is Euclidean without transformation. Colour lines join the sites in their geographic sequence along the course of the river from site 1 (headwaters) to site 30 near the junction with the Saône River.