IDEA AND PERSPECTIVE

Beta diversity as the variance of community data: dissimilarity coefficients and partitioning

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Abstract

Beta diversity can be measured in different ways. Among these, the total variance of the community data table $\mathbf{Y}$ can be used as an estimate of beta diversity. We show how the total variance of $\mathbf{Y}$ can be calculated either directly or through a dissimilarity matrix obtained using any dissimilarity index deemed appropriate for pairwise comparisons of community composition data. We addressed the question of which index to use by coding 16 indices using 14 properties that are necessary for beta assessment, comparability among data sets, sampling issues and ordination. Our comparison analysis classified the coefficients under study into five types, three of which are appropriate for beta diversity assessment. Our approach links the concept of beta diversity with the analysis of community data by commonly used methods like ordination and ANOVA. Total beta can be partitioned into Species Contributions (SCBD: degree of variation of individual species across the study area) and Local Contributions (LCBD: comparative indicators of the ecological uniqueness of the sites) to Beta Diversity. Moreover, total beta can be broken up into within- and among-group components by MANOVA, into orthogonal axes by ordination, into spatial scales by eigenfunction analysis or among explanatory data sets by variation partitioning.

Keywords

Beta diversity, community composition data, community ecology, dissimilarity coefficients, local contributions to beta diversity, properties of dissimilarity coefficients, species contributions to beta diversity, variance partitioning.

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INTRODUCTION

A most interesting property of species diversity is its organisation through space. This phenomenon, now well known to community ecologists, was first discussed by Whittaker in two seminal papers (1960, 1972) where he described the alpha, beta and gamma diversity levels of natural communities. Alpha is local diversity, beta is spatial differentiation and gamma is regional diversity. The interest of community ecologists for beta diversity stems from the fact that spatial variation in species composition allows them to test hypotheses about the processes that generate and maintain biodiversity in ecosystems. Sampling through space, time or along gradients representing processes of interest is a way of carrying out *mensurative experiments* (Hurlbert 1984) involving natural processes without the constraints (e.g. small sample size) of controlled experiments.

Beta diversity is conceptually the variation in species composition among sites within a geographical area of interest (Whittaker 1960). Several authors have used that description of the concept, including Legendre *et al.* (2005), Anderson *et al.* (2011) and Baselga & Orme (2012). Different equations have been proposed to measure that variation. Vellend (2001) and Anderson *et al.* (2011) pointed out that studies of beta diversity might focus on two aspects of community structure, distinguishing two types of beta diversity. The first is turnover, or the directional change in community composition from one sampling unit to another along a predefined spatial, temporal or environmental gradient. The second is variation in community composition among sampling units, which is a non-directional approach because it does not make reference to any explicit gradient. Both approaches are legitimate.

Regardless of whether beta diversity is defined as directional or non-directional, one can be interested in summarising it using a single number that quantifies the variation. A lot of interest has been centred on the choice of the best index to produce that number. In the directional approach, the slope of the similarity decay in species composition with geographical distance can be used as a measure of beta (Nekola & White 1999). In his 1960 paper, Whittaker suggested to compute a non-directional beta index for species richness as $\beta = \gamma/\alpha$ where γ is the number of species in the region and α is the mean number of species at the study sites within the region. Since then, several other indices have been suggested to estimate a value corresponding to beta in the turnover and non-directional frameworks; see Vellend (2001), Koleff *et al.* (2003) and Anderson *et al.* (2011) for reviews. Currently, the most popular indices belong to two families that can be labelled the additive ($H_\alpha + H_\beta = H_\gamma$) and multiplicative ($H_\alpha \times H_\beta = H_\gamma$) approaches (Jost 2007; Chao *et al.* 2012). A detailed discussion of these two families is found in a *Forum* section published by *Ecology* (2010:1962–1992).

In his introduction to the *Forum*, Ellison (2010) noted that in the additive and multiplicative approaches, beta is a derived quantity

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that is numerically related to alpha and gamma. He pointed out that it would be most useful to have a method to estimate beta diversity without prior computation of alpha and gamma; he called for computational independence, which does not imply statistical independence. The approach adopted and developed in this article is to use the total variance of the site-by-species community table **Y** as a single-number estimate of beta diversity (Pelissier *et al.* 2003; Legendre *et al.* 2005; Anderson *et al.* 2006). Fulfilling Ellison's wish, it is computed without reference to the values of alpha and gamma and its statistical dependence on gamma can be accounted for using null models (Kraft *et al.* 2011; De Cáceres *et al.* 2012). While acknowledging that other measures of beta can also achieve computational and statistical independence (e.g. Chao *et al.* 2012), one of our aims is to stress an important advantage of the total variance of **Y** over other measures: it allows ecologists to go beyond the single-number approach and partition the spatial variation in several ways to answer precise ecological questions and test hypotheses about the origin and maintenance of beta diversity in ecosystems.

We will explore the advantages and limitations of estimating beta diversity (BD_{Total}) as the total variation of the community matrix **Y**. (1) In a first section, we show that BD_{Total} can be obtained in two equivalent ways, i.e. by computing the sum-of-squares of the species occurrence or abundance data or *via* a dissimilarity matrix. When the first method is used, species abundances should be transformed in an appropriate way before computing BD_{Total}. The second method is also appealing because it allows the estimation of beta using the dissimilarity functions that are appropriate for the analysis of community data. (2) There are, however, many different dissimilarity coefficients, and not all of them are appropriate for estimating beta diversity. A comparative analysis of 16 coefficients is undertaken in the next section to guide users faced with the problem of choosing a coefficient. (3) We then present an example to illustrate the calculation of beta as the total variance of **Y** and the contributions of individual species and sampling units. (4) Following that, we show that the proposals

of Whittaker (1972) and Ricotta & Marignani (2007) are special cases of BD_{Total} computed from a dissimilarity matrix, and that the beta diversity statistic of Anderson *et al.* (2006) is closely related to BD_{Total}. (5) Finally, we show that the total variance of **Y** links beta diversity assessment with the description (through ordination) and hypothesis testing (through regression and canonical analysis) phases of community ecology, as well as other variance partitioning methods.

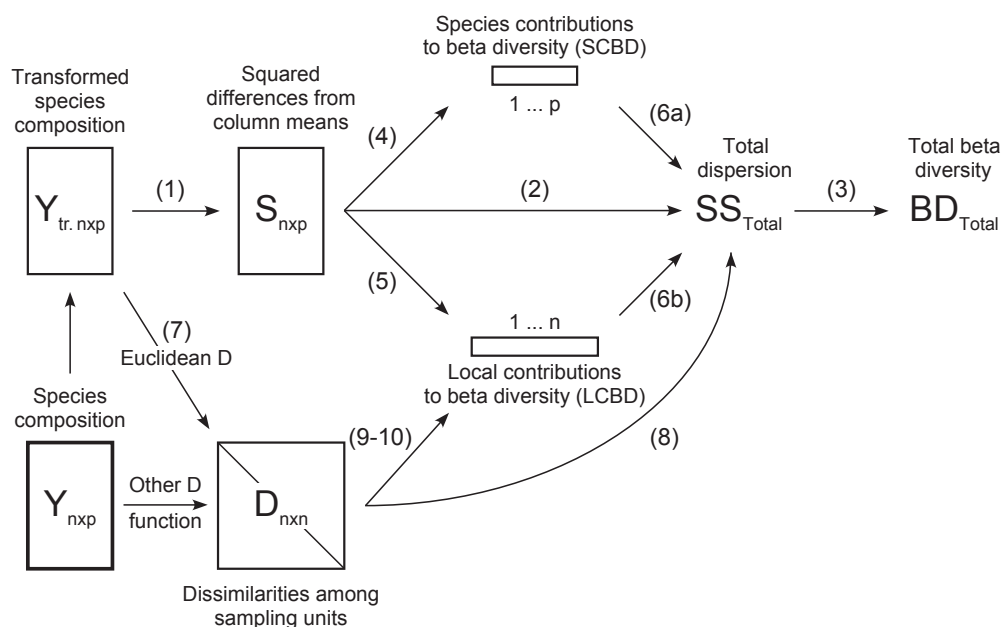## BETA DIVERSITY AS THE TOTAL COMMUNITY COMPOSITION VARIANCE

Equivalent ways of computing Var(Y)

This section presents two equivalent ways of computing the total variance of the community composition matrix **Y**. The first one is straightforward, it is simply the total variance of matrix **Y**. The second one is based on community dissimilarity matrices computed using the indices developed by ecologists over more than a century. The section also shows that the total variance can be divided into the contributions of individual species and individual sampling sites. Readers can follow the explanation on the diagram in Fig. 1.

Let **Y** = [y_{ij}] be a data table containing the presence-absence or the abundance values of p species (column vectors $\mathbf{y}_1$, $\mathbf{y}_2$, ... $\mathbf{y}_p$ of **Y**) observed in n sampling units (row vectors $\mathbf{x}_1$, $\mathbf{x}_2$, ... $\mathbf{x}_n$ of **Y**). We will use indices i and h for sampling units, index j for species and y_{ij} for individual values in **Y**. The total variance of **Y**, noted Var(**Y**), can be computed as follows:

Sums of squares
The usual way to obtain Var(**Y**) consists in computing a matrix of squared deviations from the column means. Let **S** (for 'square') be a $n \times p$ rectangular matrix where each element s_{ij} is the square of the difference between the y_{ij} value and the mean value of the corresponding jth species:

Figure 1 Schematic diagram representing the different ways of computing beta diversity as the total variance in the species composition data table **Y**, as well as the contributions of individual species and sampling units. Numbers in parentheses refer to equations in the text.

$$s_{ij} = \left(y_{ij} - \bar{y}_j\right)^2. \tag{1}$$

All s_{ij} values in column j are zero if all sites have the same abundance for species j. If we sum all values of **S**, we obtain the total sum of squares (SS) of the species composition data:

$$SS_{Total} = \sum_{i=1}^{n} \sum_{j=1}^{p} s_{ij}. \tag{2}$$

This quantity forms the basis of BD_{Total}, which is the index of beta diversity whose properties are studied in this article:

$$BD_{Total} = Var(\mathbf{Y}) = SS_{Total}/(n-1). \tag{3}$$

Equation 3 converts the sum of squares into the usual unbiased estimator of the variance, whose values can be compared between data matrices having different numbers of sampling units. SS_{Total} and $Var(\mathbf{Y}) = BD_{Total}$ were both proposed by Legendre *et al.* (2005) as measures of beta diversity. The two indices are equally useful to compare repeated surveys of a region involving the same sites, or for simulation studies, but there is a clear advantage in using $Var(\mathbf{Y})$ for comparisons among regions.

Although we advocate using $Var(\mathbf{Y})$ as a measure of beta diversity, it is important to note that eqns 1–3 should not be computed directly on raw species abundance or biomass data. Because calculating $Var(\mathbf{Y})$ on raw species abundances entails that the dissimilarity between sites is assessed using the Euclidean distance (eqn 7) and this coefficient is not appropriate for compositional data (see section 'Dissimilarity coefficients and beta assessment'), species abundance data should be transformed in an ecologically meaningful way before BD_{Total} is calculated using eqns 1–3.

An advantage of conceiving beta as the total variation in **Y** is that SS_{Total} allows the assessment of the *contributions of individual species* and of *individual sampling units to the overall beta diversity*. That is, one can compute the sum of squares corresponding to the *j*th species,

$$SS_j = \sum_{i=1}^{n} s_{ij} \tag{4a}$$

which is the contribution of species j to the overall beta diversity. SS_j divided by $(n-1)$ is the variance of species j. The *relative* contribution of species j to beta, which we call *Species Contribution to Beta Diversity* (SCBD), is thus:

$$SCBD_j = SS_j/SS_{Total}. \tag{4b}$$

In an analogous way, one can compute the sum of squares corresponding to the *i*th sampling unit,

$$SS_i = \sum_{j=1}^{p} s_{ij}. \tag{5a}$$

The SS_i values represent a genuine partitioning of beta diversity among the sites. Because the s_{ij} values are squared deviations from the species means, SS_i is the squared distance of sampling unit i to the centroid of the distribution of sites in species space. SS_i also measures the leverage of site i in a principal component analysis (PCA) ordination. The *relative* contribution of sampling unit i to beta diversity, which we call *Local Contribution to Beta Diversity* ($LCBD_i$), is thus:

$$LCBD_i = SS_i/SS_{Total}. \tag{5b}$$

LCBD values can be mapped, as will be shown in the ecological illustration below. Ecologically, they represent *the degree of uniqueness of the sampling units in terms of community composition*. Mapping the centred values using different symbols or colours is a way to highlight the sites with LCBD values higher and lower than the mean.

LCBD indices can be tested for significance by random, independent permutations within the columns of matrix **Y**; testing the $LCBD_i$ is the same as testing the SS_i indices. This permutation method tests H_0 that the species are distributed at random, independently of one another, among the sites, while preserving the species abundance distributions found in the observed data. However, it destroys the association of the species to the site ecological conditions, as well as the spatial structure of community composition resulting from assembly processes (e.g. dispersal, environmental filtering). Note that the species richness (alpha diversity) of the sites is changed by this permutation method; species-poor sites become richer in most permutations and species-rich sites become poorer. Arguably, these two kinds of sites may have large LCBD for that reason, so this permutation method includes randomisation of species richness in its null hypothesis. Other null hypotheses may be tested using other permutation schemes, e.g. by preserving site attributes such as total species richness or number of individuals (e.g. in De Cáceres *et al.* 2012). A simulation study that we performed showed that the LCBD test described here has correct rates of type I error for all coefficients that are suitable for beta diversity study (identified in section 'Comparative study').

Hence, the two decompositions of SS_{Total} are

$$SS_{Total} = \sum_{j=1}^{p} SS_j \quad \text{and} \quad SS_{Total} = \sum_{i=1}^{n} SS_i. \tag{6a, b}$$

Dissimilarity

As mentioned above, there is an alternative path starting from **Y** and leading to SS_{Total} (Fig. 1). That is, SS_{Total} can also be obtained from an $n \times n$ symmetric dissimilarity matrix $\mathbf{D} = [D_{hi}]$ containing Euclidean distances among points, computed using the classical Euclidean distance formula:

$$D_{hi} = D(\mathbf{x}_h, \mathbf{x}_i) = \sqrt{\sum_{j=1}^{p} \left(y_{hj} - y_{ij}\right)^2}. \tag{7}$$

The following equivalence is described in Legendre *et al.* (2005) and in Legendre & Legendre (2012, chapter 8):

$$SS_{Total} = \frac{1}{n} \sum_{h=1}^{n-1} \sum_{i=h+1}^{n} D_{hi}^2. \tag{8}$$

That is, one can obtain SS_{Total} by summing the squared distances in the upper or lower half of matrix **D** and dividing by the number of objects n (*not* by the number of distances). This equality (eqn 8) is demonstrated in appendix 1 of Legendre & Fortin (2010).

The Euclidean distance has long been known to be inappropriate for the analysis of community composition data (see next section). For that reason, eqns 7–8 should not be used to compute SS_{Total} unless species abundance data have been appropriately transformed so that the resulting dissimilarity assessments are ecologically meaningful (e.g. using the Hellinger or chord transformations described in Appendix S1 in Supporting Information). Equation 8 can also be generalised to distance matrices obtained using other dissimilarity indices. These indices may or may not have the Euclidean property (P13 below), but their other properties may make them appropriate for beta diversity assessment. Thus, a valid method to calculate BD_{Total} consists in computing a dissimilarity matrix **D** using a selected ecological dissimilarity coefficient instead of the Euclidean distance, and applying eqn 8 to obtain SS_{Total}, followed by eqn 3. That eqn 8

applies to ecological dissimilarities that have the Euclidean property, or not, is shown in Appendix S2. How to choose an appropriate dissimilarity coefficient for a given study is described in the next section.

It is possible to calculate the contributions of individual sampling units from **D**. Indeed, the algebra of principal coordinate analysis (PCoA, Gower 1966) offers a way of computing the sum of squares SS_i, corresponding to each sampling unit i, directly from **D**. In PCoA, prior to eigen-decomposition, the distance matrix is transformed into matrix $\mathbf{A} = [a_{hi}] = \left[-0.5D_{hi}^2 \right]$, then centred as proposed by Gower (1966) using the equation

$$\mathbf{G} = \left(\mathbf{I} - \frac{\mathbf{11}'}{n} \right) \mathbf{A} \left(\mathbf{I} - \frac{\mathbf{11}'}{n} \right) \tag{9}$$

where **I** is an identity matrix of size n, **1** is a vector of ones (length n) and **1**' is its transpose (Legendre & Legendre 2012; eqns 9.40 and 9.42). The diagonal elements of matrix **G** are the SS_i values, or the squared distances of the points to the multivariate centroid of **Y**, which is located at the centroid of the principal coordinate space:

$$[SS_i] = \operatorname{diag}(\mathbf{G}) \tag{10a}$$

The vector of local contributions of the sites to beta diversity ($LCBD_i$) is computed as follows:

$$[LCBD_i] = \operatorname{diag}(\mathbf{G})/SS_{\text{Total}}. \tag{10b}$$

Despite its advantages, working from matrix **D** instead of the matrix of squared centred values **S** entails the drawback that one looses track of the species. Because **D** is computed among sampling units over all species, the contributions of individual species cannot be recovered from **D**.

To summarise:

(1) The community data table **Y** should be transformed in an appropriate way before beta diversity is computed. One can then compute the total sum of squares in the community data **Y**, SS_{Total}, from either the transformed community composition matrix **Y** (eqns 1 and 2) or from a Euclidean distance matrix **D** computed from the transformed data (eqns 7 and 8). The two modes of calculation produce the same statistic, SS_{Total}, and from it one can compute the total variance, $BD_{\text{Total}} = \operatorname{Var}(\mathbf{Y})$ (eqn 3).
(2) Alternatively, one can use eqn 8 to compute SS_{Total} from a dissimilarity matrix **D** obtained using any appropriate dissimilarity coefficient (next section). Equation 8 applies to ecological dissimilarity indices that have the Euclidean property, or not, as demonstrated in Appendix S2.
(3) The contribution of the ith sampling unit to the overall beta diversity can be computed using eqn 5a. From these, *Local Contribution to Beta Diversity* (LCBD) coefficients can be derived. LCDB coefficients are comparative indicators of the ecological uniqueness of the sites in terms of community composition. The SS_i values are also found on the diagonal of matrix **G** (eqns 9 and 10a). The relative contributions (LCDB) are computed using eqns 5b and 10b.
(4) If BD_{Total} is calculated from **Y** (eqn 3) transformed in an appropriate way, the contribution of species j to the overall beta diversity, SS_j, is computed using eqn 4a, and the relative contributions, called the *Species Contributions to Beta Diversity* (SCBD), are computed using eqn 4b. SCBD coefficients represent the degree of variation of individual species across the study area. SS_j and SCDB coefficients cannot be derived from a distance matrix.

DISSIMILARITY COEFFICIENTS AND BETA ASSESSMENT

Since the description of the first floristic similarity coefficient by Paul Jaccard (1900), community ecologists have developed a broad array of similarity and dissimilarity coefficients. Ecologists are often faced with the question: Which community data transformation and/or (dis)similarity coefficient should I use in my study? When assessing beta diversity through the variation in community composition, one needs to specify what is meant by 'variation in community composition'. The answer will determine the choice of a community data transformation and/or dissimilarity measure, and must be carefully articulated (Anderson *et al.* 2006).

There is no single coefficient that is appropriate in all occasions. Choice should be guided by the properties of coefficients and the objective of the research. Several studies have compared resemblance coefficients, focusing on their linearity and resolution along simulated gradients (e.g. Bloom 1981; Hajdu 1981; Gower & Legendre 1986; Faith *et al.* 1987; Legendre & Gallagher 2001), or investigating theoretical properties (e.g. Janson & Vegelius 1981; Hubálek 1982; Wilson & Shmida 1984; Gower & Legendre 1986; Koleff *et al.* 2003; Chao *et al.* 2006; Clarke *et al.* 2006). Complementing these studies, we present in this section a comparative review of several abundance- and incidence-based dissimilarity coefficients, listed in Table 1. Our aim is to determine which coefficients are the most appropriate for assessing beta diversity under the present approach. We restricted the list to the coefficients originally designed for pairwise comparisons, thus excluding multiple-site dissimilarity measures (e.g. Baselga 2010, 2013). In addition, we focused on properties that are easy to understand and interpret ecologically, with preference for those that could be checked unequivocally.

Properties of dissimilarity indices for the study of beta diversity

Fourteen properties, divided into four groups, are described in Appendix S3, which also outlines procedures to check which dissimilarity indices possess them. The first two groups (P1–P9) contain the minimum requirements for assessing beta diversity. The remaining two groups (P10–P14) are not necessarily required in all beta diversity studies. Practitioners should determine whether the context of their analyses requires these properties, or not. Other properties are also considered interesting by authors of other studies on dissimilarity coefficients.

The dissimilarity coefficients

A selection of 16 quantitative dissimilarity coefficients commonly used for beta diversity assessment was considered in our comparison study. They represent a broad hand among the available coefficients. Equations are shown in Table 1 for community composition abundance and for presence–absence (i.e. incidence) data. Table 2 indicates which dissimilarity coefficients possess the properties mentioned in the previous paragraph and described in Appendix S3, as well as their maximum values (D_{max}) when they exist.

The first coefficient in the list is the Euclidean distance. Although this distance is known to be inappropriate for the analysis of community composition data sampled under varying environmental conditions (Orlóci 1978; Legendre & Gallagher 2001), it is included in

Table 1 Dissimilarity coefficients compared in this article

Dissimilarity	Abundance-based	Incidence-based	References	Coefficient no. in L&L*
Euclidean distance	$\sqrt{\sum_{j=1}^{p}\left[y_{1j}-y_{2j}\right]^2}$	$\sqrt{p\left(\dfrac{b+c}{a+b+c+d}\right)}=\sqrt{b+c}$		D_1
Manhattan distance	$\sum_{j=1}^{p}\left|y_{1j}-y_{2j}\right|$	$p\left(\dfrac{b+c}{a+b+c+d}\right)=b+c$		D_7
Modified mean character difference	$\dfrac{1}{pp}\sum_{j=1}^{p}\left|y_{1j}-y_{2j}\right|$	$\dfrac{b+c}{a+b+c}$	Legendre & Legendre (2012)	D_{19}
Species profile distance	$\sqrt{\sum_{j=1}^{p}\left[\dfrac{y_{1j}}{y_{1+}}-\dfrac{y_{2j}}{y_{2+}}\right]^2}$	$\sqrt{\dfrac{b+c}{(a+b)(a+c)}}$	Legendre & Gallagher (2001)	D_{18}
Hellinger distance	$\sqrt{\sum_{j=1}^{p}\left[\sqrt{\dfrac{y_{1j}}{y_{1+}}}-\sqrt{\dfrac{y_{2j}}{y_{2+}}}\right]^2}$	$\sqrt{2\left(1-\dfrac{a}{\sqrt{(a+b)(a+c)}}\right)}$	Rao (1995)	D_{17}
Chord distance	$\sqrt{\sum_{j=1}^{p}\left[\dfrac{y_{1j}}{\sqrt{\sum_{k=1}^{p}y_{1k}^2}}-\dfrac{y_{2j}}{\sqrt{\sum_{k=1}^{p}y_{2k}^2}}\right]^2}$	$\sqrt{2\left(1-\dfrac{a}{\sqrt{(a+b)(a+c)}}\right)}$	Orlóci (1967)	D_3
Chi-square distance	$\sqrt{y_{++}\sum_{j=1}^{p}\dfrac{1}{y_{+j}}\left[\dfrac{y_{1j}}{y_{1+}}-\dfrac{y_{2j}}{y_{2+}}\right]^2}$	NA†	Lebart & Fénelon (1971)	D_{16}
Coefficient of divergence	$\sqrt{\dfrac{1}{pp}\sum_{j=1}^{p}\left(\dfrac{y_{1j}-y_{2j}}{y_{1j}+y_{2j}}\right)^2}$	$\sqrt{\dfrac{b+c}{a+b+c}}$	Clark (1952)	D_{11}
Canberra metric‡	$\dfrac{1}{pp}\sum_{j=1}^{p}\dfrac{\left|y_{1j}-y_{2j}\right|}{(y_{1j}+y_{2j})}$	$\dfrac{b+c}{a+b+c}$	Lance & Willams (1967), Stephenson *et al.* (1972) for $1/pp$	D_{10}
Whittaker's index of association	$\dfrac{1}{2}\sum_{j=1}^{p}\left|\dfrac{y_{1j}}{y_{1+}}-\dfrac{y_{2j}}{y_{2+}}\right|$	$\dfrac{1}{2}\left(\dfrac{b}{a+b}+\dfrac{c}{a+c}+\left|\dfrac{a}{a+b}-\dfrac{a}{a+c}\right|\right)$	Whittaker (1952)	D_9
Percentage difference (*alias* Bray–Curtis dissimilarity§)	$\dfrac{\sum_{j=1}^{p}\left|y_{1j}-y_{2j}\right|}{y_{1+}+y_{2+}}$	$\dfrac{b+c}{2a+b+c}$	Odum (1950)	D_{14}
Wishart coefficient = (1−similarity ratio)	$1-\left[\dfrac{\sum_{j=1}^{p}y_{1j}y_{2j}}{\sum_{j=1}^{p}y_{1j}^2+\sum_{j=1}^{p}y_{2j}^2-\sum_{j=1}^{p}y_{1j}y_{2j}}\right]$	$\dfrac{b+c}{a+b+c}$	Wishart (1969), Janssen (1975)	

(continued)

Table 1. (continued)

Dissimilarity	Abundance-based	Incidence-based	References	Coefficient no. in L&L*
D = (1−Kulczynski coefficient)	$1 - \frac{1}{2}\left[\dfrac{\sum_{j=1}^{p} \min(y_{1j}, y_{2j})}{y_{1+}} + \dfrac{\sum_{j=1}^{p} \min(y_{1j}, y_{2j})}{y_{2+}}\right]$	$1 - \frac{1}{2}\left(\dfrac{a}{a+b} + \dfrac{a}{a+c}\right)$	Kulczynski (1928)	$1 - S_{18}$
Abundance-based Jaccard¶	$\left(1 - \dfrac{UV}{U+V-UV}\right)$	$\dfrac{b+c}{a+b+c}$	Chao et al. (2006)	
Abundance-based Sørensen¶	$\left(1 - \dfrac{2UV}{U+V}\right)$	$\dfrac{b+c}{2a+b+c}$	Chao et al. (2006)	
Abundance-based Ochiai¶	$\left(1 - \sqrt{UV}\right)$	$\left(1 - \dfrac{a}{\sqrt{(a+b)(a+c)}}\right)$	Chao et al. (2006)	

*L&L: Legendre & Legendre (2012).
†NA: No binary form with parameters a, b and c for this coefficient, although it can be computed for presence-absence data.
‡Division by pp (number of species excluding double zeros) introduced by Stephenson et al. (1972) and adopted by Oksanen et al. (2012).
§Coefficient first described by Steinhaus in the 1940s, then by Odum (1950) as the *percentage difference*. The Bray & Curtis (1957) paper described a new ordination method; the index described and used by these authors was Whittaker's dissimilarity, not the percentage difference which is more general. It is incorrect to attribute this coefficient to these authors.
¶U and V notation: see Chao et al. (2006).

the comparison where it will serve as a reference point. It is the failure of the Euclidean distance to correctly account for beta diversity (it lacks properties P4, P5, P7–P9) that makes it necessary for ecologists to rely on the other dissimilarity measures investigated in this article. The Euclidean distance may, however, become appropriate after transformation of the community data (Appendix S1). Likewise, the Manhattan distance is inappropriate *per se*; nevertheless, it is included in the comparison because it becomes the Whittaker dissimilarity after profile transformation of **Y**, and that index is appropriate for beta diversity studies (Whittaker 1952; Faith *et al.* 1987; Appendix S1).

The other coefficients included in the comparative study are double-zero asymmetric (property P4); they have been recommended and used for community composition assessment or beta diversity studies. Four of these dissimilarities can be computed using the formula in Table 1 or through the alternative method corresponding to property P14. For the species profile, Hellinger, chord and chi-square distances, the data are first transformed using the same-name transformation (Appendix S1); computing the Euclidean distance (eqn 7) on the transformed data produces the targeted profile, Hellinger, chord or chi-square distance.

When applied to presence-absence data, several quantitative coefficients in Table 1 produce either the one-complement of the Jaccard similarity index or the one-complement of the Sørensen index. The Hellinger and chord distances both produce $D = \sqrt{2(1 - \text{Ochiai similarity})}$.

Comparative study

The properties of the selected coefficients were coded into a data matrix with the coefficients as rows and properties P4–P14 as columns (Table 2). Most properties were coded as presence–absence (0–1), except for P13 which was coded on a semiquantitative 0-1-2 scale (0 = not Euclidean, 1 = $\mathbf{D}^{(0.5)}$ is Euclidean, 2 = $\mathbf{D}^{(0.5)}$ and $\mathbf{D}$ are Euclidean). The missing value in Table 2 (coded 'NA') was transformed to 1; the reason is that the chi-square distance has property P7, so it would likely have P10 if a binary form was available for that coefficient. The data matrix was subjected to PCA of the correlation matrix.

The analysis produced an ordination of the dissimilarities (Fig. 2) where similar coefficients are close to one another and dissimilar ones are more distant. Properties P4–P14, which are the variables of the matrix subjected to PCA, are shown as red arrows. One can identify five types of coefficients using the data in Table 2 and the ordination diagram:

Type I contains the Euclidean and Manhattan distances, as well as the mean character difference and the species profile distance. They all lack several of the important properties in the first two classes (P4–P9). Most notably, the Euclidean and Manhattan distances do not have the double-zero asymmetry property (P4), and the four coefficients fail to give the largest dissimilarity values to pairs of sites without species in common (P5). The distance between species profiles decreases when the number of unique species in the compared sites increases (P6). The Euclidean distance, Manhattan distance and species profile distances are not species-replication invariant (P7). Moreover, the Euclidean, Manhattan and modified mean character difference do not fulfil P8 and P9. The species profile distance is invariant to the measurement units of the data (P8), but the upper bound of $\sqrt{2}$ is only reached when there is

Table 2 Properties P4–P14 of the coefficients in Table 1. P1–P3 (not shown) are fulfilled by all coefficients. Property descriptions are found in Appendix S3. 1 indicates that a coefficient has the property, 0 that it does not. For P13, code 2 indicates that both $\mathbf{D}$ and $\mathbf{D}^{(0.5)}$ are Euclidean, 1 that only $\mathbf{D}^{(0.5)} = \left[D_{hi}^{0.5}\right]$ is Euclidean, and 0 that neither $\mathbf{D}$ nor $\mathbf{D}^{(0.5)}$ is Euclidean. NA: there is no binary form for the chi-square distance, hence P10 could not be assessed. Last column: maximum possible dissimilarity value ($D_{\max}$) when it exists. P1–P9 are essential properties for beta assessment; P10–P14 describe additional properties, useful for special applications

Dissimilarity	P4	P5	P6	P7	P8	P9	P10	P11	P12	P13	P14	$D_{\max}$
Euclidean distance	0	0	1	0	0	0	0	0	0	2	1	—
Manhattan distance	0	0	1	0	0	0	0	0	0	1	0	—
Modified mean character difference	1	0	1	1	0	0	1	0	0	0	0	—
Species profile distance	1	0	0	0	1	1	0	1	0	2	1	$\sqrt{2}$
Hellinger distance	1	1	1	1	1	1	1	1	0	2	1	$\sqrt{2}$
Chord distance	1	1	1	1	1	1	1	1	0	2	1	$\sqrt{2}$
Chi-square distance	1	0	1	1	1	1	NA	0	0	2	1	$\sqrt{2y_{++}}$
Coefficient of divergence	1	1	1	1	1	1	1	0	0	2	0	1
Canberra metric	1	1	1	1	1	1	1	0	0	1	0	1
Whittaker's index of association	1	1	1	1	1	1	1	1	0	1	0	1
Percentage difference (*alias* Bray–Curtis)	1	1	1	1	1	1	1	0	0	1	0	1
Wishart coefficient = (1−similarity ratio)	1	1	1	1	1	1	1	0	0	1	0	1
D = (1−Kulczynski coefficient)	1	1	1	1	1	1	1	0	0	0	0	1
Abundance-based Jaccard	1	1	1	1	1	1	1	1	1	0	0	1
Abundance-based Sørensen	1	1	1	1	1	1	1	1	1	0	0	1
Abundance-based Ochiai	1	1	1	1	1	1	1	1	1	0	0	1

a single, unique species per site; with more species, the maximum distance decreases with the number of unique species. Due to these shortcomings, the four coefficients belonging to type I do not allow proper assessment and comparison of beta diversity estimates among data sets.

Coefficients in types II–IV provide asymmetrical treatment of double zeros (P4) and they all have properties P5–P9, which are required for comparability of beta estimates among data sets. They are thus all appropriate for beta diversity assessment.

Type II contains the Hellinger and chord distances. These two distances are closely related: the Hellinger distance is equal to the chord distance computed on square-root-transformed species frequencies. They share all properties in classes 1 and 2, which are necessary for beta diversity assessment. Furthermore, type II coefficients are Euclidean (P13) and they can be emulated by transformations of the raw frequency or biomass data (P14). Hence, $\mathbf{D}$ matrices computed using these coefficients are fully suitable for ordination by principal coordinate analysis (PCoA), which will not produce negative eigenvalues and complex axes. For an easier and more informative ordination, species frequency (or frequency-like, such as biomass) data transformed using the Hellinger and chord transformations (Appendix S1) can be analysed directly by PCA and by canonical redundancy analysis (RDA); this is not the case for the type III and IV coefficients. (PCoA of Hellinger and chord distance matrices produces the same ordinations as PCA of the Hellinger and chord transformed data.) Moreover, SS_{Total} corresponding to the Hellinger and chord distances can be obtained by computing the transformation in Appendix S1, then applying eqns 1 and 2 to the transformed data. This is simpler than computing the distance matrix and using eqn 8 to obtain SS_{Total}. Furthermore, the Hellinger and chord transformed data allow the computation of SCBD statistics (eqn 4b), which cannot be obtained from a distance matrix.

Type III contains the divergence, Canberra, Whittaker, percentage difference (*alias* Bray–Curtis), Wishart and Kulczynski dissimilarities. They share properties (P1-P9), which are necessary for beta diversity assessment. The coefficient of divergence, which is Euclidean, can be used directly in PCoA ordination. For four coefficients (Canberra, Whittaker, percentage difference and Wishart), the square root of the distances must be taken before they are used in PCoA. The matrix of principal coordinates can be used as the response data in RDA; this is the distance-based RDA method proposed by Legendre & Anderson (1999). Among the six coefficients in this group, only the Whittaker index is invariant to the total abundance of each sampling unit (P11); the remaining indices are thus affected to some extent by differences in total abundances between the two compared sites. The Kulczynski coefficient is suitable for beta diversity assessment, but not for ordination, and it does not correct for undersampling. Considering the properties analysed in this article, this coefficient does not offer any particular advantage not available in other coefficients; it is thus not recommended for general use.

Type IV contains the abundance-based quantitative forms of the Jaccard, Sørensen and Ochiai indices. Like coefficients of type II, type IV coefficients fulfil property P11 (invariance to total abundance in individual sampling unit). In addition, they have property P12 (correction for undersampling), but not properties P13 and
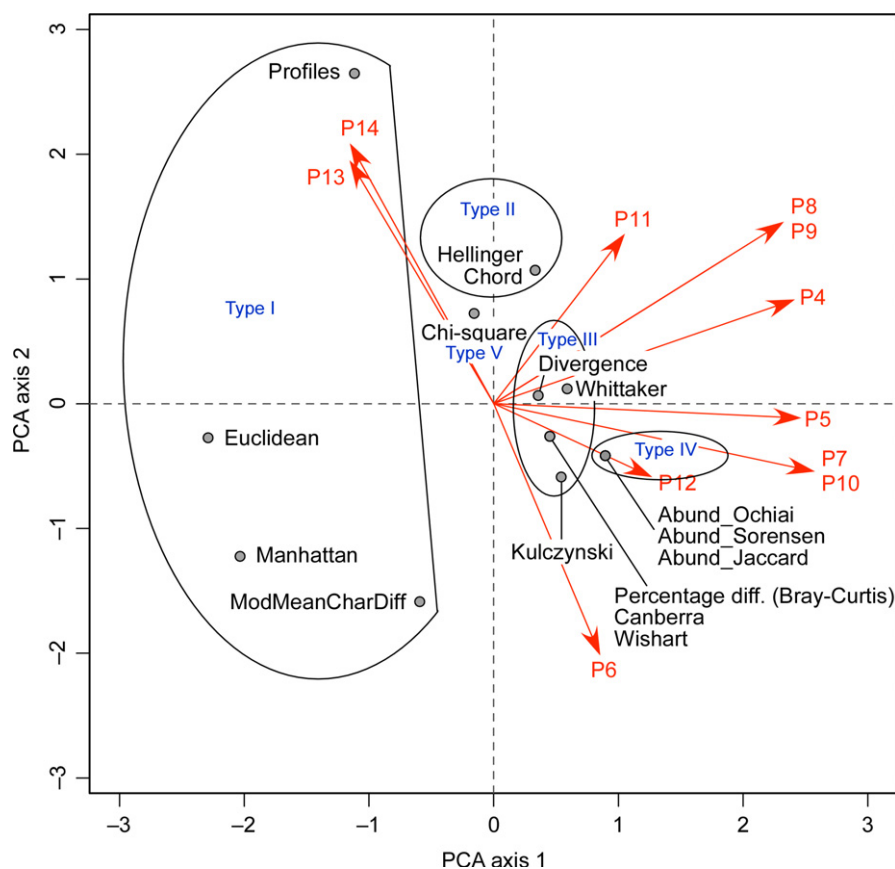
Figure 2 Principal component biplot relating properties P4–P14 (red arrows) to the dissimilarity coefficients (grey points; see Table 1 for the full coefficient names). The five types of coefficients (blue labels), shown in the figure, are described in the text. PCA axis 1 accounts for 46% of the multivariate variation and axis 2 for 23%.

P14, which are desirable for ordination. In particular, type IV coefficients are not Euclidean (P13) in quantitative form, although the Jaccard, Sørensen and Ochiai similarities, which are their binary counterparts, produce coefficients that have the Euclidean property when transformed to $D = \sqrt{1 - \text{similarity}}$ (Legendre & Legendre 2012, table 7.2).

The chi-square distance forms type V. This distance is widely used to analyse communities since it is the basis for correspondence analysis. The chi-square distance gives more importance to rare than common species in the assessment of the distance between sites, the rare species (when their abundances are correctly estimated by sampling) being considered more important indicators of special environmental conditions prevailing at some sites. Unfortunately, it lacks property P5, and this makes it unsuitable for beta diversity studies.

Maximum value of BD

All dissimilarities in types II–IV have a maximum value, reached when two sites have completely different community compositions. For example, the Hellinger and chord distances in type II have a minimum value of 0 and a maximum of $\sqrt{2}$ (Table 2). If all sites have entirely different species compositions, all $n(n-1)/2$ distances in $\mathbf{D}$ are $\sqrt{2}$ and eqns 8 and 3 produce $BD_{Total} = 1$. Hence, for these two dissimilarity indices, BD_{Total} is in the range [0, 1]. All other indices that are appropriate for beta assessment (types III and IV) have maximum values of 1. When all sites have different spe-

cies compositions, the distances are all equal to 1 and BD_{Total} computed through eqns 8 and 3 is 0.5, so that BD_{Total} is in the range [0, 0.5]. For these distances, multiplying BD_{Total} by 2 would directly produce relative BD values (BD_{rel}, Appendix S3, property P9) in the range [0, 1]. Hence, BD_{Total} has a fixed range of values for any community, which does not depend on the total abundance in the community composition table.

ECOLOGICAL ILLUSTRATION: FISH BETA DIVERSITY IN DOUBS RIVER

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 article, Verneaux proposed to use fish communities to characterise 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 geographical coordinates and environmental data (source: http://www.bio.umontreal.ca/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. As in that book, we subjected the fish data to a chord transformation before analysis (Appendix S1).

SS_{Total} (eqn 2) was 15.243 and BD_{Total} (eqn 3) was 0.544 for the fish data. The local contributions of individual sites were computed; the values of SS_i (eqn 5a) ranged from 0.291 to 0.971. An ordination diagram (Fig. 3) illustrates the mathematical meaning of SS_i
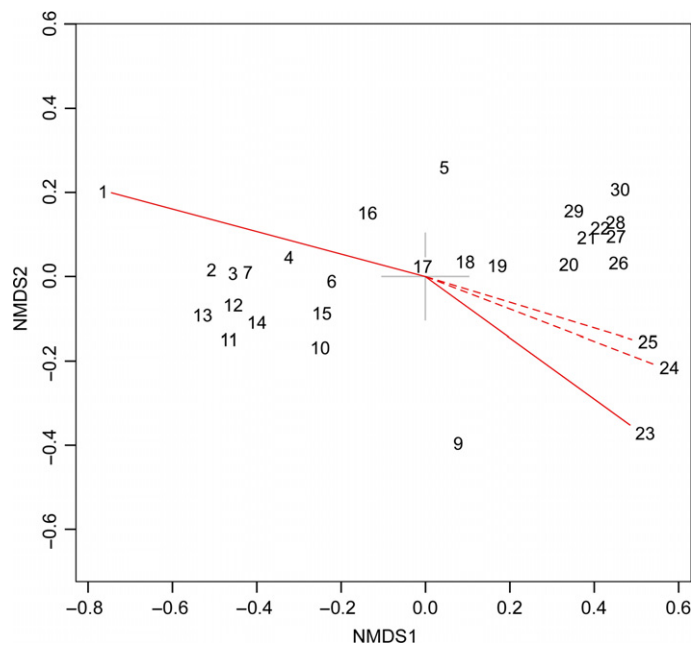
Figure 3 Ordination diagram of Doubs River fish data sites (nonmetric multidimensional scaling, nMDS; chord distance). SS_i indices are the squares of the distances of the sites to the multivariate centroid. The significant indices ($P < 0.05$) are represented by red lines joining the points to the centroid (full lines: $P < 0.05$ after Holm correction for 29 simultaneous tests).

indices: they are the squares of the distances of the sites to the multivariate centroid, as discussed under eqn 9.

The relative contributions ($LCBD_i = SS_i/SS_{Total}$, eqn 5b) were in the range [0.019, 0.064]. LCBD indices indicate the uniqueness of the fish community at each site. They are plotted on a schematic map of the river in Fig. 4a, which also shows the two sites where LCBD was statistically significant. Comparison with species richness (Fig. 4b) showed that for this data, LCBD was negatively correlated to richness ($r = -0.60$), indicating that high LCBD (i.e. high uniqueness of species composition) was often related to a small number of species. This is not, however, a general or obligatory relationship.

Environmental variables were also available for each site: distance from the source, altitude, riverbed slope, mean minimum discharge, pH, concentrations in calcium, phosphate, nitrate, ammonium and dissolved oxygen and biochemical oxygen demand (BOD). The LCBD values were regressed on the environmental variables to determine the factors that make LCBD vary along the river (adjusted $R^2 = 0.58$). Only two environmental variables were retained by backward elimination in regression: riverbed slope and BOD. Both variables had positive coefficients in the model, indicating that sites with high BD_{Total} either had a large slope (specially true at the headwaters) or were strongly eutrophic (high BOD). Note that regressing LCBD values on environmental variables is not the same as canonical analysis of the community data. For the chord-transformed Doubs fish data, forward selection of environmental variables in RDA produced a different model (adjusted $R^2 = 0.61$) containing five significant variables at the 0.05 level: distance from the source, altitude, slope, dissolved oxygen and BOD. The question in RDA is to identify the factors driving the observed variation in community composition; RDA truly analyses beta diversity by decomposing the total variance of the species data, i.e. BD_{Total}, into explained and residual components. In contrast, in regression analysis of the LCBD indices,
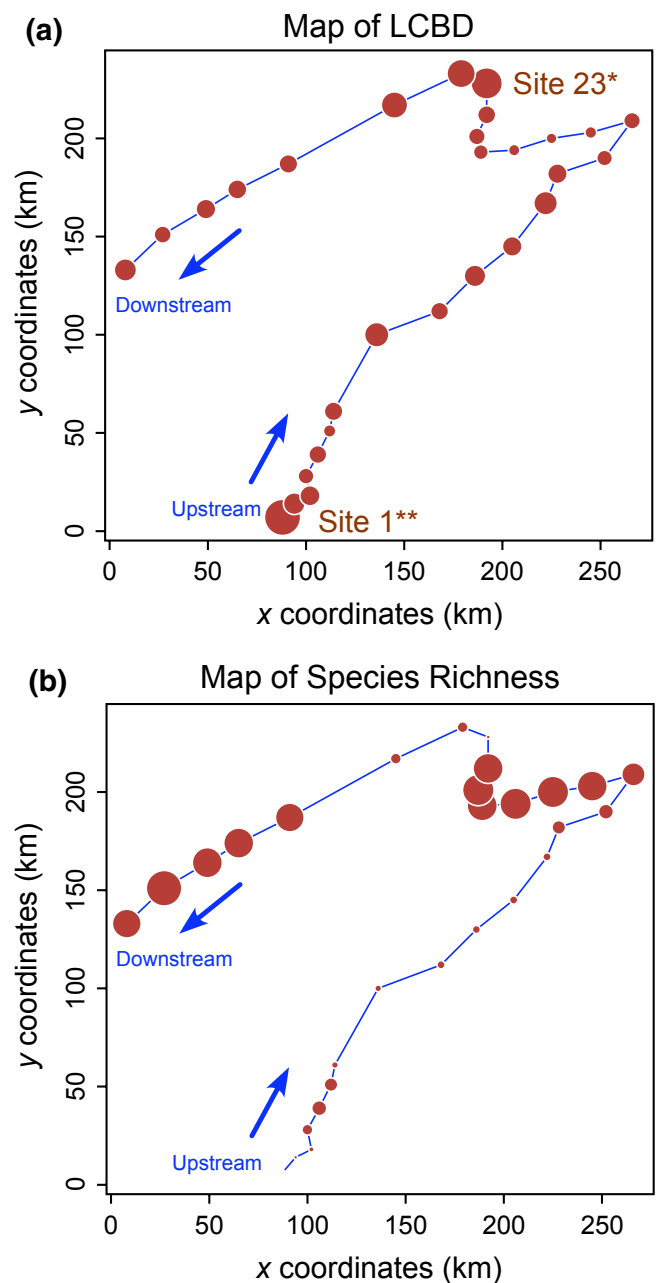
Figure 4 Maps of Doubs River (blue line) showing (a) the local contributions to beta diversity (LCBD) of the fish assemblage data and (b) the species richness at the 29 study sites. Size of the circles is proportional to the LCBD or richness values. Two sites have significant LCDB (or SS_i) indices at the 0.05 significance level after Holm correction for multiple testing: site 1 ($P = 0.003$) and site 23 ($P = 0.042$). The arrows indicate flow direction.

the question is why some sites have higher degrees of uniqueness in species composition than others.

Four species contributed to beta diversity well above the mean of the 27 species: the stone loach (*Barbatula barbatula*, Balitoridae), the common bleak (*Alburnus alburnus*, Cyprinidae), the Eurasian minnow (*Phoxinus phoxinus*, Cyprinidae), and the brown trout (*Salmo trutta fario*, Salmonidae) which had the highest SCBD index. The chord-transformed abundances of these species varied the most among sites. The brown trout, Eurasian minnow and stone loach are found

in the unpolluted sites with high LCBD upriver, which have high conservation status, whereas the common bleak is abundant in the eutrophic sites with agricultural pollution in the middle course of the river. Sites in the latter group, which also have high LCBD values, are in need of restoration.

One may wonder: For the coefficients that are appropriate for beta diversity studies, are the LCBD estimates similar or very different? Using the software in Appendix S4, calculation of LCBD was repeated for the 11 dissimilarities belonging to types II–IV, which are appropriate for beta assessment. The 11 LCBD vectors were quite similar: their mean Spearman correlation was 0.905. Kendall concordance analysis (Legendre 2005) showed that the contributions of all 11 vectors to the concordance of the group were significant. (These are not genuine tests of significance since the LCBD vectors were all computed from the same data; the concordance results provide, however, a clustering validation criterion.) These results show that LCDB indices computed using all dissimilarities that were suitable for beta diversity assessment were highly concordant.

DISCUSSION

Different concepts of beta diversity

We will first address the appropriateness of using 'beta diversity' to designate the approach described in this article. We acknowledge that this is an unsettled issue. Authors, e.g. Anderson *et al.* (2011), have rightfully argued that there are several meanings and measures associated with the concept of beta diversity. Authors agree that alpha and beta diversities are essentially different; alpha measures how diversified the species are within a site, i.e. in a single row of the site-by-species data table $\mathbf{Y}$, whereas beta measures how diversified the sites are in species composition within a region, i.e. the variation among the rows of $\mathbf{Y}$. Some ecologists prefer to reserve the expression beta diversity for the additive or multiplicative approaches, and we will not dispute their choice.

However, if beta diversity can be seen as 'the variation in species composition among sites', as stated by many authors, then the variance of $\mathbf{Y}$, which specifically measures that variation, certainly qualifies as a measure of beta. The literature is growing that adopts this broader concept and measure of beta, because it links the ecological concept of beta diversity to methods of analysis that can be applied to test hypotheses about the mechanisms that generate and maintain beta diversity in ecosystems (subsection 'Multiple ways of partitioning total beta diversity'). Those who prefer to limit the meaning of beta diversity to the additive or multiplicative approaches do not deny that variation in species composition among sites can be analysed, and hypotheses tested, but they prefer to call that variation by some other name, e.g. compositional heterogeneity among sites. Compositional heterogeneity – be it called beta diversity, or not – measures community differentiation, which results from evolutionary and ecological processes operating at several spatial (from site to global) and temporal scales.

After proposing the concept in his seminal papers, Whittaker (1960, 1972) detailed different measures of beta diversity. One of his measures corresponds precisely to the variance of $\mathbf{Y}$ measured through some dissimilarity coefficients, as will be shown in the next subsection. We are in good company here. Ecologists largely agree with Whittaker (1972) that beta diversity conceptually corresponds to *the variation in species composition among sites in the geographical region of inter-*

est. (Whittaker used a slightly different expression, 'the extent of differentiation of communities along habitat gradients'. He was interested in the response of communities to environmental variation, hence his interest for ordination methods.) Legendre *et al.* (2005) were perhaps the first to use precisely that expression, based on their reading of Whittaker, and they were followed in its use by many authors, including Anderson *et al.* (2006, 2011). Leaving the terminological issue aside, we may discuss what are the different ways of estimating the variation in species composition among sites, or beta diversity. For example, Baselga (2013) suggested calculating multiple-site dissimilarity coefficients to measure variation in species composition between more than two sites, instead of using an average of pairwise dissimilarity values. Alternative estimation methods are not in opposition but complementary; each one offers a different way of explaining beta diversity, or expressing it in a way that makes it useful for ecological interpretation, impact assessment or conservation studies. Future studies should focus on comparing alternative estimation approaches in order to clarify their differences and domains of application.

Related approaches to beta diversity assessment

In this article, we used the total variance of $\mathbf{Y}$ as an estimate of beta diversity (BD$_{\text{Total}}$) for a region of interest (eqn 3, Fig. 1). Var($\mathbf{Y}$) should not be computed using raw abundance data but after some appropriate transformation of the community composition data, or through a carefully selected dissimilarity function. The values of BD$_{\text{Total}}$ are comparable among data sets having the same or different numbers of sampling units (n), provided that the sampling units are of the same size or represent the same sampling effort, and that the calculations have been done using the same index chosen among those that have been found to be suitable for beta diversity assessment in this article. Depending on the index, BD$_{\text{Total}}$ may have a maximum value of 1 or 0.5 when all sites under study have different species compositions.

Alternative equations to estimate total BD have been proposed by Whittaker (1972), Ricotta & Marignani (2007) and Anderson *et al.* (2006). We will now show that these proposals are special cases of eqn 3 or are related to it.

In section 'Equivalent ways of computing Var($\mathbf{Y}$)', we saw that SS($\mathbf{Y}$) can be computed as the sum of the squared dissimilarities divided by n (eqn 8). This is appropriate for the Euclidean distance and for dissimilarities that have the property of being Euclidean (P13). Appendix S2 shows that SS$_{\text{Total}}$ can also be computed in that way for dissimilarities that do not lead to a fully Euclidean representation; these will not concern us in the present paragraph. Several dissimilarities, coded 1 for P13 in Table 2, are Euclidean only when taking their square roots; the square-rooted distances form matrix $\mathbf{D}^{(0.5)} = \left[D_{hi}^{0.5} \right]$. That group includes the Canberra metric, Whittaker's index, the percentage difference (*alias* Bray–Curtis) and Wishart's coefficient. Many of the incidence-based (i.e. binary) coefficients are also in that situation, including the widely used Jaccard, Sørensen and Ochiai coefficients (Legendre & Legendre 2012, table 7.2). We will show here that the method of calculation of beta diversity proposed in other papers is equivalent to DB$_{\text{Total}}$ of the present paper if $\mathbf{D}^{(0.5)}$ is used for the calculation.

(a) Whittaker (1972, p. 233) stated that 'The mean CC [Jaccard or Sørensen coefficient of community] for samples of a set compared with one another in all possible directions is one expression [of] their relative dissimilarity, or beta differentiation'. The mean is

obtained by summing the dissimilarities and dividing by the number of dissimilarities in the half-matrix, $n(n-1)/2$. This is equivalent to computing eqns 8 and 3 on the square-rooted dissimilarities (matrix $\mathbf{D}^{(0.5)}$) and multiplying by 2. Hence, Whittaker's formula only differs by a factor 2 from $\mathrm{DB_{Total}}$ computed from $\mathbf{D}^{(0.5)}$.

(b) There is also a relationship between the equation for $\mathrm{DB_{Total}}$ used in this article and the suggestion of Ricotta & Marignani (2007) to estimate beta diversity by Rao's (1982) quadratic entropy, $Q = \sum_{h=1}^{n-1}\sum_{i=h+1}^{n}\delta_{hi}p_hp_i$, where p_i and p_h contain the relative abundances of sampling units i and h in the data table, respectively, and δ_{hi} is the dissimilarity between i and h computed with any measure of one's choice. If all sampling units are considered equally important, say $p_i = 1/n$, then $Q = \frac{1}{n^2}\sum_{h=1}^{n-1}\sum_{i=h+1}^{n}\delta_{hi}$, which is very close to $\mathrm{DB_{Total}}$ computed from $\mathbf{D}^{(0.5)}$ through eqn 8 followed by eqn 3. The difference is that the last division is by n in Q instead of $(n-1)$ in eqn 3.

(c) The beta diversity statistic developed by Anderson *et al.* (2006) belongs to the same family as $\mathrm{DB_{Total}}$. It is the *sum of the dissimilarities from the sampling units to the group centroid* in multivariate space divided by n, producing a maximum likelihood estimate of the variance. It differs from $\mathrm{DB_{Total}}$, which is the *sum of the squared dissimilarities from the sampling units to the group centroid* divided by $(n-1)$ (eqn 3). The squared dissimilarities from the sampling units to the group centroid are found in vector $[\mathrm{SS}_i]$ obtained by eqns 9 and 10a computed from $\mathbf{D}$. Because it can be computed from any dissimilarity matrix, the Anderson *et al.* (2006) statistic can be computed from $\mathbf{D}$ or $\mathbf{D}^{(0.5)}$, both producing a different statistic than $\mathrm{DB_{Total}}$.

Regarding the choice of a dissimilarity measure and the equivalence of the beta diversity approaches described in the last paragraphs, different situations should be considered. (1) For dissimilarity measures that are not Euclidean for $\mathbf{D}$ but are Euclidean for $\mathbf{D}^{(0.5)}$, then the approaches of Whittaker (1972) and Ricotta & Marignani (2007) are essentially equivalent to the calculation of $\mathrm{DB_{Total}}$ in this article. (2) If the dissimilarity measure can be obtained by applying a transformation to the original data (Appendix S1) followed by the computation of the Euclidean distance, the equivalence between these methods holds in the transformed space and $\mathrm{BD_{Total}}$ can be computed by applying eqns 2 and 3 to the transformed data. (3) If the dissimilarity measure cannot be obtained by applying a transformation to the original data followed by Euclidean distance calculation, the distances to the centroid can still be computed using the square root of eqn 10a. This result holds for non-Euclidean embeddable dissimilarities as well, although with some additional complexities (Anderson 2006; Appendix S2).

Multiple ways of partitioning total beta diversity

The strongest advantage of adopting the present approach to the analysis of beta diversity lies in the possibility of partitioning the total sum-of-squares of the community composition data into additive components. The total variance is the basic currency of many statistical methods, univariate and multivariate, through which Var (**Y**) can be partitioned in different ways. Available partitioning methods include the following.

Contributions of individual species
The $\mathrm{SS_{Total}}$ statistic can be partitioned into species contributions to beta diversity (SCBD_j, eqn 4b). SCBD indices can, in principle, be

computed for raw or transformed abundance data, but it should in practice be limited to data subjected to the Hellinger or chord transformations, which are the only two that correspond to distances suitable for beta assessment. After centring, the SCBD values have signs which indicate the species that vary more (or less) than the mean across the sites. A mathematical limitation restrains the use of SCBD coefficients: they can only be computed from raw or transformed data tables with species in columns; they cannot be computed from a $\mathbf{D}$ matrix. Calculating SCBD indices is useful to determine which species exhibit large variations across the study area. Note that SCBD indices do not have the same interpretation as indicator species for groups of sites (Dufrêne & Legendre 1997; De Cáceres & Legendre 2009). The sites where species with large SCBD values are abundant and dominate the community will normally also have large LCBD indices, as we found in our example.

Contributions of individual sampling units
Likewise, the $\mathrm{SS_{Total}}$ statistic can be partitioned into local contributions of individual sampling units to beta diversity (LCBD_i, eqn 5b or 10b). The LCBD values, which can be mapped, indicate the sites that contribute more (or less) than the mean to beta diversity. LCBD are comparative indicators of site uniqueness; hence, large LCBD values indicate sites that have strongly different species compositions. For conservation biology, large LCBD values may indicate sites that have unusual species combinations and high conservation value, or degraded and species-poor sites in need of ecological restoration. They may also correspond to special ecological conditions or result from the effect of invasive species on communities. LCBD may be inversely correlated with species richness, as in our example, but in other ecosystems large LCBDs may indicate rare species combinations that are worth studying in more detail.

In data analysis, sites with high LCBD may be removed before simple or canonical ordination because they may have an undue influence on the results. This may prove a useful criterion to remove sites prior to ordination, instead of other criteria like low species richness.

Within- and among-group contributions
Groups of sites may be known *a priori* from the sampling design, or they may be obtained by clustering based on the environmental variables. For these groups of sites, the total sum-of-squares of the species data can be divided by multivariate analysis of variance (computed using MANOVA or canonical analysis) into within- and among-group sums of squares. Alternatively, groups of sites where the species respond in the same way to environmental variables can be identified by multivariate regression tree analysis.

Simple and canonical ordination
The total sum-of-squares, which estimates beta diversity, can be partitioned into orthogonal axes by simple ordination methods (PCA, CA, PCoA). Alternatively, $\mathrm{SS_{Total}}$ can be partitioned by canonical analysis (RDA or CCA) into orthogonal axes related to the environmental variables.

Contributions of sets of explanatory factors
$\mathrm{SS_{Total}}$ can be partitioned as a function of different sets of explanatory variables by variation partitioning (Borcard *et al.* 1992; Peres-Neto *et al.* 2006). Partitioning can be done, e.g. between different sets of environmental variables, or between explanatory matrices representing environmental and spatial variables (e.g. sets of spatial

eigenfunctions), depending on the hypotheses under study. This is a major approach for estimating the relative contributions of groups of explanatory variables representing different hypotheses about the origin of beta diversity.

Spatial scales

SS_{Total} can be partitioned as a function of spatial scales by spatial eigenfunction analysis. See Legendre & Legendre (2012) for a review of these methods. These and other methods of multivariate multiscale analysis were also reviewed by Dray *et al.* (2012).

Multivariate variogram and multiscale ordination

SS_{Total} can also be partitioned into spatial scales by multivariate variogram analysis (Wagner 2003). Furthermore, the species–environment relation, which represents a portion of SS_{Total}, can be partitioned into spatial scales by multiscale ordination; see Wagner (2003, 2004) and Legendre & Legendre (2012).

Choosing a dissimilarity index for beta diversity assessment

Analysing the spatial variation in species composition necessarily implies choosing a dissimilarity coefficient, either implicitly or explicitly (Legendre *et al.* 2005; Anderson *et al.* 2006). Choosing an appropriate coefficient is crucial to ensure the interpretation of the results and allow the comparison of beta diversity estimates among regions and types of organisms.

In this article, we studied several properties of coefficients, separating those that were purely mathematical from those that had an ecological interpretation. This conceptual separation was important to help users make choices on ecological grounds. Comparison of the 16 selected dissimilarity coefficients based on 14 ecological, statistical and mathematical properties led to a model where the coefficients were divided into five main types. Three of those types are suitable for beta diversity studies and comparison of beta diversity estimates computed from different ecological data sets. These different types of coefficients can be used to address different questions.

Among the unsuitable coefficients are the Manhattan and Euclidean distances. As shown in this article, these distances are appropriate for beta diversity assessments only after transformation of the raw abundance data. In the case of the Manhattan distance (L1 norm), the natural transformation is the division of each value by the total abundance, which leads to the Whittaker coefficient. In the case of the Euclidean distance (L2 norm), the natural transformation is the division of each value by the norm of the row vector, which leads to the chord distance. The Hellinger distance is the chord distance computed on square-root-transformed abundance data.

When choosing a coefficient, users should check the properties the coefficient has, and determine whether they are suitable for the objectives of the study. Further research is needed about the mathematical and ecological properties of dissimilarity coefficients and the situations where these properties are desirable or needed.

AUTHORSHIP

The two authors contributed equally to the article and took the lead at different times. PL co-ordinated the writing and editing of the final version of the manuscript.

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SUPPORTING INFORMATION

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Appendix S1

COMMUNITY COMPOSITION DATA TRANSFORMATIONS

The following data transformations (Legendre & Gallagher 2001), applied to species frequency data (or frequency-like data such as biomass) before computing the Euclidean or Manhattan distance, produce distance coefficients that are included in our comparative study:

- Species profile transformation: $y'_{ij} = y_{ij}/y_{i+}$;

- Hellinger transformation: $y'_{ij} = \sqrt{y_{ij}/y_{i+}}$;

- Chord transformation: $y'_{ij} = y_{ij}\Big/\sqrt{\sum_{j=1}^{p} y_{ij}^2}$;

- Chi-square transformation:

$$y'_{ij} = \sqrt{y_{++}}\,\frac{y_{ij}}{y_{i+}\sqrt{y_{+j}}} \quad \text{where } y_{i+} = \sum_{j=1}^{p} y_{ij}, \ \ y_{+j} = \sum_{i=1}^{n} y_{ij}, \text{ and } y_{++} = \sum_{i=1}^{n}\sum_{j=1}^{p} y_{ij}.$$

After computation of the Euclidean distance, the corresponding dissimilarities are the species profile, Hellinger, chord, and chi-square distances. The Hellinger and chord distances are appropriate for beta diversity studies, but the distance between species profiles and the chi-square distance are not; see *Comparative study* in the main paper.

Before calculation of the Euclidean or Manhattan distance, another approach is to transform community composition data using simple transformations. Examples are the usual square-root and $y'_{ij} = \log(y_{ij} + c)$ transformations (constant c is usually 1 when transforming species frequency data, but it could take other values for biomass data for example), or the special log transformation of Anderson *et al.* (2006), which makes allowance for species frequencies of

zeros. Log transformations are appropriate for species data with log-normal distribution; log-transformed data can then be used as input into the percentage difference and Kulczynski dissimilarities. Other transformations that are appropriate for community composition data were described by Faith *et al.* (1987), among other authors.

The Euclidean distance computed on data transformed using the square-root, $\log(y_{ij} + c)$, or Anderson's log transformations still lacks properties P4, P5, P7, P8 and P9 that are essential for beta diversity assessment (Appendix S3). These transformations do not solve the problems of the Euclidean distance computed on raw abundance data (Table 2).

Community composition data transformed following any of the transformations described in this section can be used in linear models such as simple (PCA) and canonical (RDA) ordination, *K*-means partitioning, and multivariate regression tree analysis (MRT); these methods implicitly preserve the Euclidean distance among sites.

Computing the Manhattan distance on data transformed into species profiles produces Whittaker's index of association multiplied by 2, which is an appropriate coefficient for beta diversity studies (Whittaker 1952). The Manhattan distance is, however, not the distance implicit in linear models, so that Whittaker's index of association does not lend itself to linear modelling nor to the calculation of *Species Contributions to Beta Diversity* (SCDB indices) described in the main paper, eqn. 4b.

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Appendix S2

COMPUTING THE TOTAL SUM OF SQUARES FROM A DISSIMILARITY MATRIX

Equation 8 in the main paper shows how to compute the total sum of squares, SS_{Total}, for a matrix of Euclidean distances. The equivalence of eq. 2 (computed on raw data) and eq. 8 (computed on distances) was demonstrated in Appendix 1 of Legendre & Fortin (2010). The profile, chord, Hellinger, and chi-square distances are obtained by first transforming the raw abundance data as described in Appendix S1, then computing the Euclidean distance formula on the transformed data. As a consequence, for these distances computed using the Euclidean distance formula, it is clear that SS_{Total} can be computed either from the transformed data through eq. 2 or from the distances through eq. 8.

For the other distances that have the Euclidean property as either $\mathbf{D}$ or $\mathbf{D}^{(0.5)} = [D_{hi}^{0.5}]$ (Table 2, column P13, codes 1 or 2), eq. 8 also applies. That point is demonstrated as follows: any dissimilarity matrix that has the Euclidean property can be decomposed into principal coordinates by principal coordinate analysis (PCoA, Gower 1966), obtaining a fully Euclidean representation of the data (Gower & Legendre 1986). Calculation of dissimilarity matrix $\mathbf{D}$ followed by PCoA of $\mathbf{D}$ or $\mathbf{D}^{(0.5)}$ acts as a data transformation. The total sum of squares of the matrix of principal coordinates, computed through eq. 2, is equal to the total sum of squares computed from dissimilarity matrix $\mathbf{D}$ or $\mathbf{D}^{(0.5)}$ through eq. 8.

Finally, for dissimilarities that do not lead to a fully Euclidean representation (i.e. those that do not have the Euclidean property; Table 2, column P13, code 0), the same equivalence still exists although these matrices produce negative eigenvalues in PCoA. The demonstration involves two steps. On the one hand, the trace of the Gower-centred matrix on which eigen-

decomposition is computed, which is equal to the sum of all eigenvalues (positive and negative), is equal to SS_{Total} computed from the dissimilarity matrix through eq. 8. On the other hand, McArdle & Anderson (2001) and Anderson (2006) have shown how to compute SS_{Total} of the principal coordinate representation using the real and complex principal coordinates, and this is equal again to the trace of the Gower-centred matrix on which eigen-decomposition is computed in PCoA. Their method has three steps: (1) square all values in the matrix of eigenvectors (which were produced by eigen-decomposition with a norm of 1), (2) multiply each squared eigenvector by its eigenvalue, and (3) sum all the resulting values. The calculation is demonstrated in the R function pcoa.short() in R, below.

Illustration: calculation of SS_{Total} for a non-Euclidean dissimilarity matrix

For the example, we will use the first 10 rows of the mite data available in package **vegan** and compute the percentage difference dissimilarity. The calculations are done in the R language.

```
require(vegan)
data(mite)

### Compute the percentage difference dissimilarity for the mite data (first 10 rows)
mite.D <- vegdist(mite[1:10,], "bray")
# Is the dissimilarity matrix Euclidean?
require(ade4)
is.euclid(mite.D)                                    # Available in R package ade4
# [1] FALSE

### Compute SS_Total from the dissimilarities

SS.D <- function(D, n) sum(D^2) / (n)                # Equation 8
res.SS.D <- SS.D(mite.D, 10)
res.SS.D
# [1] 0.9626073                                      # Result: SS_Total

### A short function for principal coordinate analysis (PCoA)

################################################################################
pcoa.short <- function(D, include.zero=FALSE, only.values=FALSE)
#
# Compute PCoA for a Euclidean or non-Euclidean dissimilarity matrix.
```

```
# The eigenvectors are not scaled to sqrt(eigenvalues),
# hence they are not principal coordinates in the PCoA sense.
#
# When 'n' is very large, users may choose not to compute the eigenvectors.
# This is obtained by selecting the option only.values=TRUE.
# The statistic VarTotal=SS will not be computed and printed in that case.
#
# License: GPL-2
# Author:: Pierre Legendre
{
      D <- as.matrix(D)
      n <- nrow(D)
      epsilon <- sqrt(.Machine$double.eps)
#
# Gower centring, matrix formula
      One <- matrix(1,n,n)
      mat <- diag(n) - One/n
      G <- -0.5 * mat %*% (D^2) %*% mat
      trace <- sum(diag(G))
      SSi <- diag(G)
#
# Eigenvalue decomposition
      eig <- eigen(G, symmetric=TRUE, only.values=only.values)
# Exclude the null eigenvalue/s if include.zero is FALSE
      select <- 1:n
      exclude <- which(abs(eig$values) < epsilon)
      cat("Note - Eigenvalue/s", exclude, "is/are null\n")
      if(!include.zero) {
            cat("Note - Eigenvalue/s and eigenvector/s", exclude, "was/were excluded\n")
            select <- select[-exclude]
            }
      values <- eig$values[select]
#
if(!only.values) {                        # Compute SS from the eigenvectors
      vectors <- eig$vectors[,select]
      vectors.sq <- vectors^2 %*% diag(values)
      SS <- sum(vectors.sq)
      } else {
      vectors <- NA
      SS <- NA
      }
#
list(values=values, vectors=vectors, trace=trace, SS.total=SS, SSi=SSi, site.names=rownames(D),
select=select)
}
###############################################################################
```

```
res <- pcoa.short(mite.D)
# Note - Eigenvalue/s 9 is/are null
# Note - Eigenvalue/s and eigenvector/s 9 was/were excluded
```

Compute SS_{Total} as the trace of the Gower-centred matrix

```
res$trace
# [1] 0.9626073                                    # Result: SS_Total
```

Compute SS_{Total} as the sum of the PCoA eigenvalues

```
sum(res$values)
# [1] 0.9626073                                    # Result: SS_Total
```

Compute SS_{Total} as the sum of squares of the principal coordinates scaled to lengths equal to the square roots of the eigenvalues, including the one with a negative eigenvalue. The result is the same with options include.zero=FALSE or include.zero=TRUE.

```
res$SS.total
# [1] 0.9626073                                    # Result: SS_Total
```

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Appendix S3

DETAILS ABOUT THE PROPERTIES OF DISSIMILARITY COEFFICIENTS

We describe four groups of properties and indicate the reason why we consider them relevant. The first two groups (i.e. from P1 to P9) contain the minimum requirements for assessing beta diversity. The remaining two groups (i.e. P10 to P14) are not necessarily required in all beta diversity assessments. Practitioners should determine whether the context of their analyses requires these latter properties or not. Similarity coefficients should be transformed into dissimilarities before assessing the following properties.

Property class 1: Basic necessary properties. — Properties P1 to P6 must be fulfilled by all resemblance coefficients used for beta diversity assessment. P1 and P2 are actually mathematical axioms that define a dissimilarity function. Thus, they are fulfilled by all coefficients considered in this paper. P3 (monotonicity) is a necessary condition for any coefficient used to study species assemblages. All coefficients investigated in the present study are monotonic. Properties P1 to P3 are therefore not shown in Table 1 of the paper.

P1 – Minimum of zero and positiveness. A dissimilarity value should never be negative and it should be zero when comparing a site to itself. When comparing two different sites, it can be zero or greater than zero, depending on the species abundance values and how the dissimilarity is defined. For example, with some coefficients, D is zero when comparing two site vectors whose abundance values are proportional to each other; that is the case with the profile, chi-square, chord, and Hellinger distances. Dissimilarities that violate this property by taking negative values are called nonmetric, by opposition to the metric and semimetric coefficients (see Legendre & Legendre 2012).

P2 – Symmetry. Consider two community abundance vectors, $\mathbf{x}_1$ and $\mathbf{x}_2$, whose dissimilarity is to be assessed. In symmetric indices, $D(\mathbf{x}_1,\mathbf{x}_2) = D(\mathbf{x}_2,\mathbf{x}_1)$. In the incidence-based counterparts of these coefficients (Table 1 in the main paper), the values b and c play exchangeable (symmetric) roles. When studying beta diversity, there is no reason to make a distinction between the two sampling units that are compared using a coefficient. Therefore, dissimilarity coefficients must be symmetric. The property of being *double-zero symmetrical*, referred to in P4, is different.

P3 – Monotonicity to changes in abundance. Increasing the difference in abundances of one of several species between two sites increases their dissimilarity. Property P3 was verified using ordered comparison case series (OCCAS), corresponding to linear changes in the abundances of two species along different types of simulated environmental gradients. The OCCAS method was proposed by Hajdu (1981) and used by Gower & Legendre (1986) to assess monotonicity in dissimilarity coefficients.

P4 – Double-zero asymmetry. Coefficients that have this property do not change when double-zeros are added to the data, but the dissimilarity decreases when double-X (where X > 0) values are added. The reasoning implies two conditions, derived from ecological niche theory.

1. Ecological statement: double-zeros in species abundance are not interpretable. — In his seminal paper, Whittaker (1972) published a figure (his Fig. 4, p. 228) showing simulated species represented by bell-shaped curves with different widths (species tolerances), succeeding one another along three ecological gradients. (1.1) For species j observed at a pair of sites, the presence of that species (in any abundance) at both sites indicates that the two sites are similar to some extent, i.e. they are close in positions along the gradient. Because the two sites are within the tolerance zone of species j, that species can be found at these two sites. (1.2) Ruling out sampling error, the presence at one site and absence at the other unambiguously indicates that the

sites occupy different positions along the gradient. (1.3) Ruling out sampling error again, double absence of species j is not interpretable, because it can result from the two sites being either at close positions along the gradient but outside the tolerance zone of species j (e.g. pH too high at both sites for that species), or at positions far away along the gradient, both sites being outside the tolerance zone of species j (e.g. pH too low at one site and too high at the other).

2. Lemma. — The presence of species j at two sites (point 1.1 above) is an indication of resemblance of these sites whatever the abundances observed. It follows that presence of species j with the same abundance X at two sites (a difference $(X - X) = 0$ for that species; point 1.1 above) has a different meaning from the double-absence (which also corresponds to a difference $(0 - 0) = 0$; point 1.3 above).

3. This reasoning leads to the following conclusions. (3.1) Double-zeros (0, 0) have a different meaning than double-presences (X, X), whatever the abundances. (3.2) Coefficients that produce the same effect (i.e. no change in dissimilarity) for double zeros as they do for double presences with identical abundances (i.e. (X,X), which we call double-X), where X > 0) are called *double-zero symmetrical* because they treat double zeros like any other pair of identical values. These coefficients are not admissible for the study of ecological differentiation of communities, i.e. for beta diversity studies. The Euclidean and Manhattan distances belong to that type: double-zeros and double-X produce no change in distance, whereas any other pair of non-identical abundances does produce a change in the distance. (3.3) Coefficients useful for beta diversity studies must be *double-zero asymmetrical* (term used in Legendre and Legendre 2012), meaning that their value does not change with the addition of double zeros, but it decreases when species with double-X abundances that are not double-zeros are added to the comparison of two sites.

The difference between double-zero and double-X is clearly recognized in binary coefficients. In double-zero symmetrical similarity coefficients such as the simple matching index, the numbers of double-presences and of double-absences (usually respectively represented by *a* and *d*) are used as indications of similarity. In contrast, double-zero asymmetrical similarity coefficients such as the Jaccard and Sørensen indices exclude double-absences (*d*) from both their numerator and denominator and use only the double-presences (*a*) in their formula in addition to *b* and *c*. Some binary dissimilarity coefficients can be expressed as function of *b* and *c* only (see, for example, the presence-absence formulas for the Euclidean and Manhattan distances in Table 1 of the main paper). These are also double-zero symmetrical, because neither double-presences (*a*) nor double-absences (*d*) can change the value of the coefficient. A double-zero asymmetrical binary dissimilarity coefficient must include double-presences (*a*) and exclude double-absences (*d*) from its formula.

P5 – Sites without species in common have the largest dissimilarity. Coefficients that violate this property are not suitable for beta diversity studies. For the coefficients that have a fixed upper bound (last column of Table 2), the largest dissimilarity is the upper bound. The following data sets were used to test the 16 coefficients analysed in this paper. In each example, the rows are sites S1-S4, the columns represent species.

Example data 1 –

	1	*2*	*3*	*4*	*5*	*6*	*7*	*8*	*9*	*10*	*11*	*12*	*13*	*14*	*15*	*16*	*17*	*18*	*19*	*20*
S1	3	7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
S2	7	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
S3	1	1	1	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0	0

S4	0	0	0	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1	1	1

Example data 2 –

	1	2	3	4
S1	1	4	0	0
S2	4	1	0	0
S3	0	1	1	0
S4	1	0	0	1

Example data 3 –

	1	2	3	4
S1	1	2	0	0
S2	2	1	0	0
S3	0	1	40	0
S4	1	0	0	40

Some dissimilarity functions present the following paradox with one of more of these data sets: for sites 3 and 4 that have no species in common, these coefficients produce dissimilarities that are smaller than for sites that have some (e.g. sites 1 and 3) or all (sites 1 and 2) their species in common. These examples are extensions of the Orlóci (1978, p. 46) paradox data.

P6 – Dissimilarity does not decrease in series of nested species assemblages. For pairs of sites having any number of unique species, i.e. species that are not found at the other site, the dissimilarity should be the same or increase with the number of unique species. In particular, the dissimilarity should not decrease when the number of unique species in one or both sites increases. To assess this property, we carried out simulations where we added unique species to one of the sites (which corresponds to the data structure described as *nestedness* of species assemblages by Wright & Reeves 1992 and Baselga 2010) or to both sites (data structure described as monotonic by Jost *et al.* 2011). Violation of P6 leads to the paradox that the total sum of squares for a pair of sites, which is $D^2/2$ (eq. 8 in the main paper), tends to 0 as the number of unique species increases.

Property class 2: Comparability between data sets. — The following three properties are needed to appropriately compare beta diversity values calculated for different data tables, even if the sampling unit are the same size (e.g. quadrat size for vegetation) and the sampling effort is the same. Therefore, we consider they should also be required in beta diversity studies.

P7 – Species replication invariance. A community composition table with the columns in two or several copies should produce the same dissimilarities among sites as the original data table. Procedure: select a community composition data table, compute a dissimilarity index and obtain a dissimilarity matrix. Then, duplicate the data table, combining the two copies side by side, using for example function cbind() in R. Compute the same dissimilarity function and obtain a new dissimilarity matrix. Repeat the duplication step to include three copies of the data and compute the dissimilarity matrix again. The three dissimilarity matrices should be identical if the dissimilarity function has the property of *replication invariance*. For the abundance-based coefficients, the property is computed using the population formula, not the sample formula. This

property was first described by Jost *et al.* (2011).

A special case of this property (not included as a separate property in the present study), for presence-absence data, is called *homogeneity*, for example by Janson and Vegelius (1981), Koleff *et al.* (2003) and Chao *et al.* (2006). The homogeneity property allows the comparison of beta values computed from data tables containing different total species richness. This property is verified on the binary form of the coefficients, by multiplying *a*, *b*, *c* and *d* by a constant factor and checking whether the resulting index value is changed.

P8 – Invariance to the measurement units. This property concerns abundance-based formulas only. It allows the comparison of beta values between data tables (e.g. regions) with different productivities (abundance or biomass), or where biomass has been measured using different units (e.g. in g and mg). To see whether a given quantitative coefficient is invariant to changes of measurement scale, we multiplied the abundance values by a constant factor and checked whether the resulting index was altered.

P9 – Existence of a fixed upper bound. The existence of an upper bound for a coefficient facilitates the interpretation and comparison of beta values because an upper bound in the dissimilarity index leads to an upper bound in the beta diversity value. The maximum beta value for a region is obtained when all site pairs have the maximum dissimilarity D_{max} permitted by the chosen coefficient. One can apply eq. 8 to that situation to compute the maximum sum of squares:

$$\mathrm{SS}_{max} = \frac{1}{n}\left(\frac{n(n-1)}{2}D_{max}^2\right) = \frac{n-1}{2}D_{max}^2$$

then eq. 3 to obtain the maximum beta diversity value:

$$\text{BD}_{\max} = \text{SS}_{\max}/(n{-}1) = \left(\frac{n-1}{2}D_{\max}^2\right)\frac{1}{n-1} = \frac{1}{2}D_{\max}^2$$

The upper bound varies among dissimilarity coefficients (Table 2 of the pain paper, right-hand column). For coefficients with $D_{\max} = \sqrt{2}$, $\text{BD}_{\max} = 1$; for those with $D_{\max} = 1$, $\text{BD}_{\max} = 0.5$ (see section "Maximum value of BD" in the pain paper). For the chi-square distance, $D_{\max} = \sqrt{2y_{++}}$ and $\text{BD}_{\max} = y_{++}$ which is the sum of the species abundances in **Y**. Although y_{++} varies from data table to data table, the chi-square distance is considered as belonging to the group of the coefficients that have a fixed upper bound because its sister index, the chi-square metric (not otherwise discussed in this paper), has an upper bound of $\sqrt{2}$ (see e.g. Legendre and Legendre 2012). The chi-square distance is the chi-square metric multiplied by $\sqrt{y_{++}}$, hence it has an upper bound of $\sqrt{2y_{++}}$. The chi-square distance is the one computed in software packages; this is why its properties are described here. The chi-square metric and distance have the same properties besides their different maximum values. Hence, for coefficients that have a fixed maximum (see section "The dissimilarity measures" in the main paper), we can compute a relative value of beta diversity, BD_{rel}, as follows:

$$\text{BD}_{\text{rel}} = \text{BD}_{\text{Total}}/\text{BD}_{\max}$$

which is a value between 0 and 1. BD_{rel} is useful to compare beta values computed using different coefficients.

Property class 3: Sampling issues. — This group of properties is mostly related to sampling issues. The fulfilment of properties P10 and P11 facilitates (but does not ensure) the comparability of beta values obtained from sampling units having different sizes or sampled using different efforts. Indeed, both the number of species and the total abundance may be

strongly affected by changes in the size of sampling units or in sampling effort. On the other hand, if the size of sampling units and sampling effort are sufficiently homogeneous, ecologists may be interested in allowing differences in the numbers of species, and perhaps also in the total abundances between sites, to influence the dissimilarity and beta diversity assessments.

The last property deals with correction for undersampling (P12) of the community composition. This property is also related to sampling effort. It is related to sampling unit size as well because small sampling units can lead to undersampling the richness of the targeted community.

P10 – Invariance to the number of species in each sampling unit. This property analyses whether a double-zero asymmetrical binary coefficient changes its value depending on the number of species in each of two sampling units x_1 and x_2 that are compared. Does the dissimilarity 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?

This property was verified algebraically on the binary form of the coefficients; it could not be checked for the chi-square metric which does not have a binary form. We start with the usual a, b, c notation for binary indices:

a = number of species shared between x_1 and x_2

b = number of unique species in x_1 that do not appear in x_2

c = number of unique species in x_2 that do not appear in x_1

We then define the number of species in x_1 and x_2 as $n_1 = a + b$ and $n_2 = a + c$, and the proportion of shared species with respect to each site as $p_1 = a / n_1 = a / (a + b)$ and $p_2 = a / n_2 = a / (a + c)$. After defining n_1, n_2, p_1 and p_2, one can reformulate the binary dissimilarity measures found in column *Incidence-based* of Table 1 of the main paper in terms of these four quantities, instead of using the notation a, b, c. The idea of the proof is to see whether a dissimilarity measure can be

reformulated using a notation that uses n_1, n_2, p_1 and p_2, and then see if these terms n_1 and n_2 cancel out in the formula. In other words, we ask whether $D(a, b, c) = D(n_1, n_2, p_1, p_2)$ can be reduced to $D(p_1, p_2)$. The following equivalences are useful for reformulation:

$$a = (a + b) \times (a / (a + b)) = n_1 \times p_1 = (a + c) \times (a / (a + c)) = n_2 \times p_2$$

$$b = (a + b) \times (1 - (a / (a + b))) = n_1 \times (1 - p_1)$$

$$c = (a + c) \times (1 - (a / (a + c))) = n_2 \times (1 - p_2)$$

Using the presence-absence form of each dissimilarity measure (column *Incidence-based* in Table 1), property P10 is verified algebraically by trying to cancel n_1 and n_2 out of the formula.

P10 is a stricter property than *homogeneity* (see P7, second paragraph). It is easy to show that fulfilling P10 leads to a coefficient that is homogeneous (invariant to the total number of species of the data set), because if $D(a, b, c) = D(p_1, p_2)$, and knowing that $p_1 = a / (a + b) = k{\cdot}a / (k{\cdot}a + k{\cdot}b)$ and $p_2 = a / (a + c) = k{\cdot}a / (k{\cdot}a + k{\cdot}c)$, then we have $D(a, b, c) = D(ka, kb, kc)$, which proves *homogeneity*. However, the reverse does not follow. Indeed, a given coefficient may be homogeneous without satisfying P10. An example is the asymmetric binary similarity coefficient proposed by Kulczynski (1928), $S_{12} = a / (b + c)$ (S_{12} in Legendre & Legendre 2012), which is homogeneous but does not fulfil P10.

Proofs for individual coefficients –

(1) **Euclidean distance**. When this distance is calculated on presence-absence data it can be formulated as:

$$E = \sqrt{b + c} = \sqrt{n_1 \cdot (1 - p_1) + n_2 \cdot (1 - p_2)}$$

Because n_1 and n_2 cannot be cancelled out, the Euclidean distance does NOT satisfy P10.

(2) **Manhattan distance**. When this distance is calculated on presence-absence data it can be formulated as:

$$M = |b + c| = |n_1 \cdot (1 - p_1) + n_2 \cdot (1 - p_2)|$$

As before, the Manhattan distance does NOT satisfy P10.

(3) **Jaccard** similarity index (proof thanks to A. Chao).

$$J = \frac{a}{a + b + c} = \frac{a}{2a + b + c - a} = \frac{n_1 p_1}{(n_1 p_1 + n_2 p_2) + n_1(1 - p_1) + n_2(1 - p_2) - n_1 p_1}$$

$$= \frac{n_1 p_1}{n_1 + n_2 - n_1 p_1} = \frac{1}{(1/p_1) + (1/p_2) - 1}$$

Thus, the Jaccard index DOES satisfy P10. All resemblance coefficients that are equal to the Jaccard index for presence-absence data satisfy P10: the **modified mean character difference**, **coefficient of divergence**, **Canberra metric**, **Wishart coefficient** (1- Similarity ratio), and **abundance-based Jaccard**.

(4) **Sørensen** similarity index (proof thanks to A. Chao) The Sørensen similarity index is

$$S = \frac{2a}{2a + b + c} = \frac{2n_1 p_1}{n_1 p_1 + n_2 p_2 + n_1(1 - p_1) + n_2(1 - p_2)}$$

$$= \frac{2n_1 p_1}{n_1 + n_2} = \frac{2}{(1/p_1) + [n_2/(n_1 p_1)]} \text{ and, since } n_1 p_1 = n_2 p_2,$$

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

Thus, the Sørensen index DOES satisfy P10. All resemblance coefficients that are equal to the Sørensen index for presence-absence data satisfy P10: the **percentage difference** and **abundance-based Sørensen**.

(5) **Ochiai** similarity index:

$$O = \frac{a}{\sqrt{(a+b)(a+c)}} = \sqrt{\frac{a}{(a+b)} \cdot \frac{a}{(a+c)}} = \sqrt{p_1 \cdot p_2}$$

Thus, the Ochiai index DOES satisfy P10. All resemblance coefficients that are equal to the Ochiai index for presence-absence data satisfy P10: the **Hellinger distance**, **chord distance**, and **abundance-based Ochiai**. In this coefficient, the similarity is the geometric mean of p_1 and p_2.

(6) **Species profile distance**. When this distance coefficient is calculated on presence-absence data, it can be written using the *a-b-c-d* notation as:

$$SP = \sqrt{\frac{b+c}{(a+b)(a+c)}}$$

After reformulating this index, we can reduce it to:

$$SP = \sqrt{\frac{n_1 \cdot (1-p_1) + n_2 \cdot (1-p_2)}{n_1 \cdot n_2}} = \sqrt{\frac{1-p_2}{n_1} + \frac{1-p_1}{n_2}}$$

Because n_1 and n_2 cannot be cancelled out, the species profile distance does NOT satisfy P10.

(7) **Whittaker's index of association**. When this distance coefficient is calculated on presence-absence data, it can be written using the *a-b-c-d* notation as:

$$W = \frac{1}{2}\left(\frac{b}{a+b} + \frac{c}{a+c} + \left|\frac{a}{a+b} - \frac{a}{a+c}\right|\right)$$

After reformulating this index, we can reduce it to:

$$W = \frac{1}{2}\left(\frac{n_1 \cdot (1-p_1)}{n_1} + \frac{n_2 \cdot (1-p_2)}{n_2} + \left|\frac{n_1 \cdot p_1}{n_1} - \frac{n_2 \cdot p_2}{n_2}\right|\right)$$

$$W = \frac{1}{2}\left((1-p_1) + (1-p_2) + |p_1 - p_2|\right) = \frac{1}{2}\left[2 - (p_1 + p_2) + |p_1 - p_2|\right]$$

Thus, the Whittaker index of association also DOES satisfy P10.

(8) **Kulczynski** similarity index. When this *similarity* is calculated on presence-absence data it can be straightforwardly formulated as:

$$K = \frac{1}{2}\left[\frac{a}{a+b} + \frac{a}{a+c}\right] = \frac{1}{2}[p_1 + p_2]$$

Thus, the Kulczynski similarity also DOES satisfy P10. In this coefficient, the similarity is the arithmetic mean of p_1 and p_2.

P11 – Invariance to the total abundance in each sampling unit. Except when researchers only count and identify a fixed number of individuals (which is often the case in plankton or palaeoecological studies), sampling units in the data table are likely to have different total abundances. Some abundance-based dissimilarity indices are only sensitive to relative abundances per site whereas others reflect differences in site total counts. This property was called "density invariance" by Jost *et al.* (2011). It is not the same as property P7 above. One can check property P11 by determining whether a coefficient is altered when the abundances are multiplied by a constant factor that is different for each sampling unit.

P12 – Coefficients with corrections for undersampling. With higher sampling effort, i.e. larger sampling units, rare species, and in particular those that are not found at the two sites under comparison, are more likely to be observed (Chao *et al.* 2006, Cardoso *et al.* 2009). For that reason, dissimilarity coefficients generally underestimate the dissimilarities among sites, the bias decreasing when sampling effort increases. For some binary similarity coefficients, Chao *et al.* (2006) and Jost *et al.* (2011) suggested abundance-based counterparts that incorporate corrections for undersampling bias.

Property class 4: Ordination-related properties. — The remaining properties are not related to the ecological interpretation of a coefficient or the comparability of beta diversity

values. They are, however, useful for ordination and linear modelling of community composition data.

P13 – Euclidean property of D or D$^{(0.5)}$. A dissimilarity matrix **D** is *Euclidean* if it can be embedded in a Euclidean space of real axes such that the Euclidean distances among points are equal to the dissimilarity values in **D**. For coefficients that are Euclidean, principal coordinate analysis of **D** produces ordinations that are fully represented in Euclidean space (i.e. without negative eigenvalues). Several coefficients have the Euclidean property. Some coefficients that are not Euclidean for **D** become Euclidean after taking the square root of the dissimilarity values (Gower & Legendre 1986); the resulting matrix, which contains values [$D_{hi}^{0.5}$], is noted **D**$^{(0.5)}$. Legendre & Legendre (2012, Tables 7.2 and 7.3) describe the Euclidean properties of 43 commonly-used similarity and dissimilarity coefficients, including several of the coefficients listed in Table 1.

P14 – Emulated by transformation of the raw frequency data followed by Euclidean distance. Legendre & Gallagher (2001) described how some distance coefficients can be obtained by computing the Euclidean distance (eq. 7 in the main paper) after transforming the raw data values in some appropriate way. Four such transformations are described in Appendix S1. Coefficients that can be obtained in that way are interesting because one can obtain BD$_{Total}$ by computing the transformation and then applying eqs 1-3. Moreover, transformed data allow the computation of the beta diversity contributions of individual species through eqs 4a and 4b (SCBD indices) and of sites through eqs 5a and 5b (LCBD indices). One can also use the transformed data directly in linear modelling of community composition data, e.g. by simple (PCA) or canonical (RDA) ordination, *K*-means partitioning, or multivariate regression tree analysis (MRT), because these methods implicitly preserve the Euclidean distance among sites.

In addition to the coefficients obtained by transformation followed by calculation of the Euclidean distance (Appendix S1), the Whittaker index can also be obtained by applying the Manhattan distance to profile transformed data; see section "The dissimilarity coefficients" in the main paper. This produces twice Whittaker's index of association; for that reason, Whittaker's index was dubbed "relativized Manhattan" by Faith *et al.* (1987). The Manhattan distance is, however, not the distance implicit in linear models, so that Whittaker's index of association does not lend itself to linear modelling nor to the calculation of *Species Contributions to Beta Diversity* (SCDB indices) described in the main paper, eq. 4b.

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Beta diversity computed as Var(Y)

Description

Compute estimates of total beta diversity as the total variance in a community data matrix **Y**, as well as derived SCBD and LCBD statistics, for 20 dissimilarity coefficients or the raw data table. Computing beta diversity as Var(**Y**) for raw, untransformed community composition data is not recommended. Tests of significance of the LCDB indices are also produced.

Usage

```
beta.div(Y,method="hellinger",sqrt.D=FALSE,samp=TRUE,nperm=999,save.D=FALSE)
```

Arguments

Y   Community composition data. The file class can be either `data.frame` or `matrix`.

method   One of the 20 dissimilarity coefficients, or "none". See Details. Names can be abbreviated to a non-ambiguous set of first letters. Default: method="hellinger".

sqrt.D   If `sqrt.D=TRUE`, the dissimilarities in matrix **D** are square-rooted before computation of SStotal, BDtotal and LCBD. This transformation may be useful for methods {"manhattan", "modmeanchardiff", "whittaker", "divergence", "canberra", "percentagedifference", "wishart"} since square-root transformation of the dissimilarities makes these **D** matrices Euclidean.
             Note 1 – Euclideanarity is useful for ordination by principal coordinate analysis; lack of this property does not adversely affect SStotal, BDtotal and LCBD.
             Note 2 – The logical value given to parameter `sqrt.D` has no incidence on calculations through methods {"euclidean", "profiles", "hellinger", "chord", "chisquare", "none"} since no **D** matrix is computed in those cases.

samp   If `samp=TRUE`, the abundance-based distances (ab.jaccard, ab.sorensen, ab.ochiai, ab.simpson) are computed for sample data. If `samp=FALSE`, they are computed for true population data.

nperm   Number of permutations for the tests of significance of LCBD indices.

save.D   If `save.D=TRUE`, the distance matrix will appear in the output list.

clock   If `clock=TRUE`, the computation time is printed. Useful when `nperm` is large.

Details

Calculations may be carried out in two ways, depending on the selected method.

• For untransformed or transformed raw data, the total sum of squares (SStotal) is first computed, then the total beta diversity (BDtotal), which is SStotal divided by (n – 1), is calculated. This algorithm is used for methods {"euclidean", "profiles", "hellinger", "chord", "chisquare", "none"}. No dissimilarity matrix nor transformation of the data is computed when the method is

"euclidean" or "none" (no transformation). For methods "profiles", "hellinger", "chord" and "chisquare", the algorithm begins with computation of the same-name transformation of the community data (Legendre and Gallagher 2001; Legendre and Legendre 2012, Section 7.7); SStotal and BDtotal are then computed for the transformed data.

• Calculations can also be conducted from a dissimilarity matrix. SStotal is computed by summing the squared dissimilarities in the lower triangular dissimilarity matrix and dividing by n; then, total beta diversity (BDtotal) is computed as above. Choices are: method = {"manhattan", "modmeanchardiff", "whittaker", "divergence", "canberra", "percentagedifference", "wishart", "kulczynski", "ab.jaccard", "ab.sorensen", "ab.ochiai", "ab.simpson", "jaccard", "sorensen", "ochiai"}. Equations for these dissimilarities are presented in Table 1 of Legendre and De Cáceres (2013). See Chao et al. (2006) for details about the abundance-based (ab) coefficients.

The Jaccard, Sørensen and Ochiai coefficients are the binary forms of 9 of the 11 dissimilarity coefficients that are suitable for beta diversity assessment. The equivalences are described in Legendre and De Cáceres (2013, Table 1). These popular coefficients can be computed directly using function beta.div() without going to the trouble of applying the quantitative forms of these coefficients to data reduced to presence-absence form. The transformation to presence-absence is done directly by function dist.binary() of package ade4, which is used by beta.div() to compute these coefficients. That function produces the dissimilarity matrix in the form sqrt(D), which is Euclidian. Hence for these three coefficients, function beta.div() should be used with option sqrt.D=FALSE.

(1) *Species contributions to beta diversity* (SCBD indices for the species) are computed for the untransformed or transformed raw data, but not for dissimilarity matrices. (2) *Local contributions to beta diversity* (LCBD indices) represent the degree of uniqueness of the sites in terms of their species compositions. They can be computed in all cases: raw (not recommended) or transformed data, as well as dissimilarity matrices. See Legendre and De Cáceres (2013) for details.

LCBD indices are tested for significance by random, independent permutations within the columns of **Y**. This permutation method tests H_0 that the species are distributed at random, independently of one another, among the sites, while preserving the species abundance distributions in the observed data. See Legendre and De Cáceres (2013) for discussion.

Value

Function beta.div returns a list containing the following results:

SStotal_BDtotal	Total sum of squares and total beta diversity [= Var(**Y**)] of the data matrix. BDtotal statistics computed with the same **D** index are comparable among data sets having the same or different numbers of sampling units (n), provided that they are of the same size or represent the same sampling effort.
SCBD	Vector of *Species contributions to beta diversity* (SCBD), if computed.
LCBD	Vector of *Local contributions to beta diversity* (LCBD) for the sites.
p.LCBD	P-values associated with the LCBD indices.
method	Method selected.
note	Notes indicate whether the selected coefficient is Euclidean or not.
D	The distance matrix if save.D=TRUE.

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License: GPL-2.

Example

```
### Example: mite data available in the vegan package
require(vegan)
data(mite)
res = beta.div(mite, "hellinger", nperm=999)

# Plot a map of the LCDB indices
# First, load the file of Cartesian coordinates of the 70 mite sampling sites
data(mite.xy)
plot(mite.xy, asp=1, type="n", xlab="x coordinates (m)", ylab="y coordinates (m)", main="Map
of mite LCBD")
points(mite.xy, pch=21, col="white", bg="brown", cex=120*res$LCBD)

### Example using the mite abundance data and the percentage difference dissimilarity
res = beta.div(mite, "percentage", nperm=999, clock=TRUE)

# Plot a map of the LCDB indices
# First, load the file of cartesian coordinates of the 70 mite sampling sites
data(mite.xy)
signif = which(res$p.LCBD <= 0.05)        # Which are the significant LCDB indices?
nonsignif = which(res$p.LCBD > 0.05)      # Which are the non-significant LCDB indices?
plot(mite.xy, asp=1, type="n", xlab="x coordinates (m)", ylab="y coordinates (m)", main="Map
of mite LCBD (red = significant indices)")
points(mite.xy[nonsignif,], pch=21, col="white", bg="blue", cex=100*res$LCBD[nonsignif])
points(mite.xy[signif,], pch=21, col="white", bg="red", cex=100*res$LCBD[signif])
```

```
beta.div <- function(Y, method="hellinger", sqrt.D=FALSE, samp=TRUE, nperm=999, save.D=FALSE,
clock=FALSE)
#
# Compute estimates of total beta diversity as the total variance in Y,
# for 20 dissimilarity coefficients or analysis of raw data (not recommended).
# LCBD indices are tested by permutation within columns of Y.
# This version includes direct calculation of the Jaccard, Sorensen and Ochiai
# coefficients for presence-absence data.
#
# Arguments --
#
# Y : community composition data matrix.
# method : name of one of the 20 dissimilarity coefficients, or "none" for
#          direct calculation on Y (also the case with method="euclidean").
# sqrt.D : If sqrt.D=TRUE, the distances in matrix D are square-rooted before
#          computation of SStotal, BDtotal and LCBD.
# samp : If samp=TRUE, the abundance-based distances (ab.jaccard, ab.sorensen,
#        ab.ochiai, ab.simpson) are computed for sample data. If samp=FALSE,
#        they are computed for true population data.
# nperm : Number of permutations for test of LCBD.
# save.D : If save.D=TRUE, the distance matrix will appear in the output list.
# clock : If clock=TRUE, the computation time is printed in the R console.
#
# License: GPL-2
# Author:: Pierre Legendre, December 2012, April-May 2013
{
### Internal functions
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
    }
###
BD.group1 <- function(Y, method, save.D, per)
    {
    if(method=="profiles") Y = decostand(Y, "total")
    if(method=="hellinger") Y = decostand(Y, "hellinger")
    if(method=="chord") Y = decostand(Y, "norm")
    if(method=="chisquare") Y = decostand(Y, "chi.square")
    #
    s <- scale(Y, center=TRUE, scale=FALSE)^2   # eq. 1
    SStotal <- sum(s)          # eq. 2
    BDtotal <- SStotal/(n-1)   # eq. 3
    if(!per) { SCBD<-apply(s,2,sum)/SStotal }else{ SCBD<-NA }  # eqs. 4a and 4b
    LCBD <- apply(s, 1, sum)/SStotal  # eqs. 5a and 5b
    #
    D <- NA
    if(!per & save.D)   D <- dist(Y)
    #
    out <- list(SStotal_BDtotal=c(SStotal,BDtotal), SCBD=SCBD, LCBD=LCBD,
    method=method, D=D)
    }
###
BD.group2 <- function(Y, method, sqrt.D)
    {
```

```
        if(method == "divergence") {
            D = D11(Y)

    } else if(any(method ==
        c("jaccard","sorensen","ochiai")))
            {
            if(method=="jaccard") D = dist.binary(Y, method=1) # ade4 takes sqrt(D)
            if(method=="sorensen")  D = dist.binary(Y, method=5) #ade4 takes sqrt(D)
            if(method=="ochiai") D = dist.binary(Y, method=7) # ade4 takes sqrt(D)

    } else if(any(method ==
        c("manhattan","canberra","whittaker","percentagedifference","wishart")))
            {
            if(method=="manhattan") D = vegdist(Y, "manhattan")
            if(method=="canberra")  D = vegdist(Y, "canberra")
            if(method=="whittaker") D = vegdist(decostand(Y,"total"),"manhattan")/2
            if(method=="percentagedifference") D = vegdist(Y, "bray")
            if(method=="wishart")   D = WishartD(Y)
            } else {
            if(method=="modmeanchardiff") D = D19(Y)
            if(method=="kulczynski")  D = vegdist(Y, "kulczynski")
            if(method=="ab.jaccard")  D = chao(Y, coeff="Jaccard", samp=samp)
            if(method=="ab.sorensen") D = chao(Y, coeff="Sorensen", samp=samp)
            if(method=="ab.ochiai")   D = chao(Y, coeff="Ochiai", samp=samp)
            if(method=="ab.simpson")  D = chao(Y, coeff="Simpson", samp=samp)
            }
        #
        if(sqrt.D) D = sqrt(D)
        SStotal <- sum(D^2)/n       # eq. 8
        BDtotal <- SStotal/(n-1)   # eq. 3
        delta1 <- centre(as.matrix(-0.5*D^2), n)   # eq. 9
        LCBD <- diag(delta1)/SStotal              # eq. 10b
        #
        out <- list(SStotal_BDtotal=c(SStotal,BDtotal), LCBD=LCBD,
        method=method, D=D)
        }
###
###
method <- match.arg(method, c("euclidean", "manhattan", "modmeanchardiff", "profiles",
"hellinger", "chord", "chisquare", "divergence", "canberra", "whittaker",
"percentagedifference", "wishart", "kulczynski", "ab.jaccard",
"ab.sorensen","ab.ochiai","ab.simpson","jaccard","sorensen","ochiai","none"))
#
if(any(method == c("profiles", "hellinger", "chord", "chisquare", "manhattan",
"modmeanchardiff", "divergence", "canberra", "whittaker", "percentagedifference",
"kulczynski"))) require(vegan)
if(any(method == c("jaccard","sorensen","ochiai"))) require(ade4)
#
if(is.table(Y)) Y <- Y[1:nrow(Y),1:ncol(Y)]    # In case class(Y) is "table"
n <- nrow(Y)
#
aa <- system.time({
if(any(method ==
c("euclidean", "profiles", "hellinger", "chord", "chisquare","none"))) {
    note <- "Info -- This coefficient is Euclidean"
    res <- BD.group1(Y, method, save.D, per=FALSE)
    #
```

```r
    # Permutation test for LCBD indices, distances group 1
    if(nperm>0) {
        p <- ncol(Y)
        nGE.L = rep(1,n)
        for(iperm in 1:nperm) {
            Y.perm = apply(Y,2,sample)
            res.p <- BD.group1(Y.perm, method, save.D, per=TRUE)
            ge <- which(res.p$LCBD >= res$LCBD)
            nGE.L[ge] <- nGE.L[ge] + 1
            }
        p.LCBD <- nGE.L/(nperm+1)
        } else { p.LCBD <- NA }
    #
    if(save.D) { D <- res$D } else { D <- NA }
    #
    out <- list(SStotal_BDtotal=res$SStotal_BDtotal, SCBD=res$SCBD,
    LCBD=res$LCBD, p.LCBD=p.LCBD, method=method, note=note, D=D)

} else {
#
    if(method == "divergence") {
        note = "Info -- This coefficient is Euclidean"
    } else if(any(method == c("jaccard","sorensen","ochiai"))) {
        note = c("Info -- This coefficient is Euclidean because dist.binary ",
        "of ade4 computes it as sqrt(D). Use beta.div with option sqrt.D=FALSE")
    } else if(any(method ==
      c("manhattan","canberra","whittaker","percentagedifference","wishart"))) {
        if(sqrt.D) {
        note = "Info -- This coefficient, in the form sqrt(D), is Euclidean"
        } else {
        note = c("Info -- For this coefficient, sqrt(D) would be Euclidean",
        "Use is.euclid(D) of ade4 to check Euclideanarity of this D matrix")
        }
    } else {
        note = c("Info -- This coefficient is not Euclidean",
        "Use is.euclid(D) of ade4 to check Euclideanarity of this D matrix")
    }
#
    res <- BD.group2(Y, method, sqrt.D)
    #
    # Permutation test for LCBD indices, distances group 2
    if(nperm>0) {
        nGE.L = rep(1,n)
        for(iperm in 1:nperm) {
            Y.perm = apply(Y,2,sample)
            res.p <- BD.group2(Y.perm, method, sqrt.D)
            ge <- which(res.p$LCBD >= res$LCBD)
            nGE.L[ge] <- nGE.L[ge] + 1
            }
        p.LCBD <- nGE.L/(nperm+1)
        } else { p.LCBD <- NA }
#
    if(sqrt.D) note.sqrt.D<-"sqrt.D=TRUE"  else  note.sqrt.D<-"sqrt.D=FALSE"
    if(save.D) { D <- res$D } else { D <- NA }
    #
    out <- list(SStotal_BDtotal=res$SStotal_BDtotal, LCBD=res$LCBD,
    p.LCBD=p.LCBD, method=c(method,note.sqrt.D), note=note, D=D)
```

```r
}
#
})
aa[3] <- sprintf("%2f",aa[3])
if(clock) cat("Time for computation =",aa[3]," sec\n")
#
class(out) <- "beta.div"
out
}

D11 <- function(Y, algo=1)
#
# Compute Clark's coefficient of divergence.
# Coefficient D11 in Legendre and Legendre (2012, eq. 7.51).
#
# License: GPL-2
# Author:: Pierre Legendre, April 2011
{
Y <- as.matrix(Y)
n <- nrow(Y)
p <- ncol(Y)
# Prepare to divide by pp = (p-d) = no. species present at both sites
Y.ap <- 1 - decostand(Y, "pa")
d <- Y.ap %*% t(Y.ap)
pp <- p-d   # n. species present at the two compared sites
#
if(algo==1) {   # Faster algorithm
    D <- matrix(0, n, n)
    for(i in 2:n) {
        for(j in 1:(i-1)) {
            num <- (Y[i,]-Y[j,])
            den <- (Y[i,]+Y[j,])
            sel <- which(den > 0)
            D[i,j] = sqrt(sum((num[sel]/den[sel])^2)/pp[i,j])
            }
        }
#
} else {   # Slower algorithm
    D <- matrix(0, n, n)
    for(i in 2:n) {
        for(j in 1:(i-1)) {
            temp = 0
            for(p2 in 1:p) {
                den = Y[i,p2] + Y[j,p2]
                if(den > 0) {
                    temp = temp + ((Y[i,p2] - Y[j,p2])/den)^2
                    }
                }
            D[i,j] = sqrt(temp/pp[i,j])
            }
        }
#
    }
DD <- as.dist(D)
}

D19 <- function(Y)
```

```r
#
# Compute the Modified mean character difference.
# Coefficient D19 in Legendre and Legendre (2012, eq. 7.46).
# Division is by pp = number of species present at the two compared sites
#
# License: GPL-2
# Author:: Pierre Legendre, April 2011
{
Y <- as.matrix(Y)
n <- nrow(Y)
p <- ncol(Y)
# Prepare to divide by pp = (p-d) = n. species present at both sites
Y.ap <- 1 - decostand(Y, "pa")
d <- Y.ap %*% t(Y.ap)
pp <- p-d    # n. species present at the two compared sites
#
D <- vegdist(Y, "manhattan")
DD <- as.dist(as.matrix(D)/pp)
}

WishartD <- function(Y)
#
# Compute dissimilarity - 1 - Wishart similarity ratio (Wishart 1969).
#
# License: GPL-2
# Author:: Pierre Legendre, August 2012
{
CP = crossprod(t(Y))
SS = apply(Y^2,1,sum)
n = nrow(Y)
mat.sq = matrix(0, n, n)
for(i in 2:n) {
    for(j in 1:(n-1)) { mat.sq[i,j] = CP[i,j]/(SS[i] + SS[j] - CP[i,j]) }
    }
mat = 1 - as.dist(mat.sq)
}

chao <- function(mat, coeff="Jaccard", samp=TRUE)
#
# Compute Chao et al. (2006) abundance-based indices.
#
# Arguments -
# mat = data matrix, species abundances
# coef = "Jaccard" : modified abundance-based Jaccard index
#        "Sorensen": modified abundance-based Sørensen index
#        "Ochiai"  : modified abundance-based Ochiai index
#        "Simpson" : modified abundance-based Simpson index
# samp=TRUE : Compute dissimilarities for sample data
#     =FALSE: Compute dissimilarities for true population data
#
# Details -
# For coeff="Jaccard", the output values are identical to those
# produced by vegan's function vegdist(mat, "chao").
#
# Help received from A. Chao and T. C. Hsieh in July 2012 for the computation
# of dissimilarities for true population data is gratefully acknowledged.
#
```

```r
# Reference --
# Chao, A., R. L. Chazdon, R. K. Colwell and T. J. Shen. 2006.
# Abundance-based similarity indices and their estimation when there
# are unseen species in samples. Biometrics 62: 361-371.
#
# License: GPL-2
# Author:: Pierre Legendre, July 2012
{
require(vegan)
nn = nrow(mat)
res = matrix(0,nn,nn)
if(samp) {   # First for sample data
for(k in 2:nn) {
    for(j in 1:(k-1)) {
        #cat("k =",k,"  j =",j,"\n")
        v1 = mat[j,]    # Vector 1
        v2 = mat[k,]    # Vector 2
        v1.pa = decostand(v1,"pa")   # Vector 1 in presence-absence form
        v2.pa = decostand(v2,"pa")   # Vector 2 in presence-absence form
        N.j = sum(v1)    # Sum of abundances in vector 1
        N.k = sum(v2)    # Sum of abundances in vector 2
        shared.sp = v1.pa * v2.pa    # Vector of shared species ("pa")
        if(sum(shared.sp) == 0) {
            res[k,j] = 1
        } else {
        C.j = sum(shared.sp * v1)    # Sum of shared sp. abundances in v1
        C.k = sum(shared.sp * v2)    # Sum of shared sp. abundances in v2
        # a1.j = sum(shared.sp * v1.pa)
        # a1.k = sum(shared.sp * v2.pa)
        a1.j = length(which((shared.sp * v2) == 1)) # Singletons in v2
        a1.k = length(which((shared.sp * v1) == 1)) # Singletons in v1
        a2.j = length(which((shared.sp * v2) == 2)) # Doubletons in v2
        if(a2.j == 0) a2.j <- 1
        a2.k = length(which((shared.sp * v1) == 2)) # Doubletons in v1
        if(a2.k == 0) a2.k <- 1
        # S.j = sum(v1[which(v2 == 1)]) # Sum abund. in v1 for singletons in v2
        # S.k = sum(v2[which(v1 == 1)]) # Sum abund. in v2 for singletons in v1
        sel2 = which(v2 == 1)
        sel1 = which(v1 == 1)
        if(length(sel2)>0) S.j = sum(v1[sel2]) else S.j = 0
        if(length(sel1)>0) S.k = sum(v2[sel1]) else S.k = 0

        U.j = (C.j/N.j) + ((N.k-1)/N.k) * (a1.j/(2*a2.j)) * (S.j/N.j) # Eq. 11
        if(U.j > 1) U.j <- 1
        U.k = (C.k/N.k) + ((N.j-1)/N.j) * (a1.k/(2*a2.k)) * (S.k/N.k) # Eq. 12
        if(U.k > 1) U.k <- 1

        if(coeff == "Jaccard") {                      # "Jaccard"
            res[k,j] = 1 - (U.j*U.k/(U.j + U.k - U.j*U.k))
            } else if(coeff == "Sorensen") {          # "Sorensen"
            res[k,j] = 1 - (2*U.j*U.k/(U.j + U.k))
            } else if(coeff == "Ochiai") {            # "Ochiai"
            res[k,j] = 1 - (sqrt(U.j*U.k))
            } else if(coeff == "Simpson") {
            # Simpson (1943), or Lennon et al. (2001) in Chao et al. (2006)
            res[k,j] = 1 -
            (U.j*U.k/(U.j*U.k+min((U.j-U.j*U.k),(U.k-U.j*U.k))))
```

```r
            } else { #
            stop("Incorrect coefficient name")
            }
        }
        }
    }

} else {    # Now for complete population data

for(k in 2:nn) {
    for(j in 1:(k-1)) {
        v1 = mat[j,]   # Vector 1
        v2 = mat[k,]   # Vector 2
        v1.pa = decostand(v1,"pa")   # Vector 1 in presence-absence form
        v2.pa = decostand(v2,"pa")   # Vector 2 in presence-absence form
        shared.sp = v1.pa * v2.pa    # Vector of shared species ("pa")
        if(sum(shared.sp) == 0) {
            res[k,j] = 1
        } else {
        N1 = sum(v1)   # Sum of abundances in vector 1
        N2 = sum(v2)   # Sum of abundances in vector 2
        U = sum(shared.sp * v1)/N1   # Sum of shared sp. abundances in v1
        V = sum(shared.sp * v2)/N2   # Sum of shared sp. abundances in v2

        if(coeff == "Jaccard") {                    # "Jaccard"
            res[k,j] = 1 - (U*V/(U + V - U*V))
            } else if(coeff == "Sorensen") {        # "Sorensen"
            res[k,j] = 1 - (2*U*V/(U + V))
            } else if(coeff == "Ochiai") {          # "Ochiai"
            res[k,j] = 1 - (sqrt(U*V))
            } else if(coeff == "Simpson") { # "Simpson"
            res[k,j] = 1 - (U*V/(U*V+min((U-U*V),(V-U*V)))) # Eq. ?
            } else { #
            stop("Incorrect coefficient name")
            }
        }
        }
    }
}
res <- as.dist(res)
}

######## End of beta.div function
```