Mathematically and biologically consistent framework for presence-absence pairwise indices of diversity

A.L. Šizling[1*], E. Tjørve[2], K.M.C. Tjørve[2], J.D. Žárský[3], P. Keil[4] and D. Storch[1,3]

[1]Center for Theoretical Study, Jilská 1, 110 00, Praha 1, Czech Republic
[2]Inland Norway University of Applied Sciences, PO Box 952, NO-2604 Lillehammer, Norway;
[3]Department of ecology, Faculty of Science, Charles University, Viničná 7, 128 44 Praha 2
[4] Faculty of Environmental Sciences, Czech University of Life Sciences Prague, Kamýcká 129, Praha – Suchdol, 16000, Czech Republic
sizling@cts.cuni.cz, storch@cts.cuni.cz.
kathy.tjorve@inn.no, even.tjorve@inn.no, jakub.dan.zarsky@gmail.com, pkeil@seznam.cz.
*corresponding author

Abstract

Aim A large number of indices that compare two or more assemblages have been proposed or reinvented. The interpretation of the indices varies across the literature, despite efforts for clarification and unification. Most of the effort has focused on interdependence between the indices and the mathematics behind them. At the same time, following issues have been underestimated: (i) the difference between statistical independence of indices and the independence based on their informational value, and (ii) the inferences from the indices about diversity patterns and phenomena. Here we offer an alternative framework for diversity indices.

Methods We distinguish different classes of dependence, and show that three indices which are mutually independent in terms of their information content are sufficient for appropriate inferences. This applies regardless of whether the indices are statistically correlated or not. We classify 20 existing indices into three main and four minor mutually independent families, and demonstrate how similarity between assemblages violates the stability of the families, confusing conceptually different patterns. We show what can be inferred about spatial diversity phenomena from different indices, demonstrate problems with most of the indices of nestedness, and show which combinations of indices may be used for meaningful ecological inference.

Results and Main conclusions We demonstrate that no single index can properly filter out a single effect of a phenomena because the phenomena inevitably bound each other (e.g. species richness gradient bounds possible values of Jaccard index of community similarity). Consequently, inventing indices which seemingly purify these effect (e.g. pure turnover or pure nestedness) leads to misleading inference. In contrast, a proper inference is obtained by using a combination of classical indices from different, mutually independent families. Our framework provides a practical clue how to compare different indices across the literature.

Key words: beta-diversity, biodiversity, co-occurrence, partitioning, dependence, Simpson, Baselga

Introduction

The effort to capture variation in biological diversity using a single variable has generated an array of approaches (e.g., Brualdi & Sanderson, 1999; Gotelli, 2000; Koleff & Gaston, 2002; Koleff *et al.*, 2003; Gaston *et al.*, 2007; Jost, 2007; Ulrich *et al.*, 2009; Baselga, 2010; Tuomisto, 2010). Differences in species occurrence in space and time are typically assessed between assemblages or species ranges by various indices. However, their application has been contentious. There is an astounding number of indices or measures to choose from, with little consensus about which are more appropriate for different purposes (e.g., Vellend, 2001; Koleff *et al.*, 2003; Jost, 2007; Juranski *et al.*, 2009; Baselga, 2010; Tuomisto, 2010; Carvalho *et al.*, 2012). The lack of consensus results from absence of a consistent framework for a proper interpretation of the indices and their mutual relationships. This has led to a repeated introduction of seemingly new indices, which in reality are mathematically equivalent to existing ones (e.g., $\beta_t = \beta_{SR} = \beta_{HK}$, defined by Wilson and Shmida 1984, Schluter and Ricklefs 1993, Harte and Kinzig 1997, respectively).

Several attempts for synthesis have been made (Koleff *et al.*, 2003; Gaston *et al.*, 2007; Jost, 2007; Tuomisto, 2010; Lyashevska & Farnsworth, 2012) and several frameworks to systemize the indices have been proposed (Jost, 2007; Baselga, 2010; Tuomisto, 2010). For example, Tuomisto (2010), and Jost (2007) show how abundance-based indices fit into the framework of Hill numbers (Hill, 1973; Chao *et al.*, 2012, 2014a, 2014b; Chiu *et al.*, 2014). However, data on abundances are rarely available, and there is a need for a consistent framework for indices based on only presences and absences (i.e., incidences). Other frameworks rarely pay attention to accurate inferences concerning ecological processes that can be obtained from different indices (but see Baselga, 2010; *Anderson et al.*, 2010).

Authors proposing new indices (e.g., Simpson, 1943; Jost, 2007; Baselga, 2007, 2010) often emphasize that they should be independent of each other, and of species richness. This independence is typically defined *statistically*, which includes the search for bounds on the y-axis imposed by the x-axis (e.g., Simpson, 1943; Baselga, 2010) or correlations between values of the indices (e.g., Koleff *et al.*, 2003; Ulrich & Gotelli, 2007; Lyashevska & Farnsworth, 2012). A finding that two indices are mutually dependent is then understood as evidence that each index captures information about two or more phenomena. This logic resulted either in the proposition of a new index, or in partitioning of an existing index to supposedly independent components, each capturing a single pattern or phenomenon (see Lennon *et al.*, 2001; Koleff & Gaston, 2002; Baselga, 2010 for examples). For example, Jaccard index depends on the difference in species richness between two focal sites (i.e., on species richness gradient, see note 5 pp. 19-20 in Simpson 1943), which has led to the definition of Simpson beta (β_{Sim}, Table 1). Baselga (2010) later pointed out that Simpson beta and Sørensen dissimilarity (β_t, Table 1) are correlated, and introduced a new index of nestedness ($\beta_{nes} \stackrel{\text{def}}{=} \beta_t - \beta_{Sim}$). The new index was based on partitioning the beta-diversity into two components (β_{nes}, and β_t), suggesting that β_{nes} and β_t are mutually independent and carry complementary information about assemblages. More specifically, Baselga (2010) suggests that high β_{nes} or β_t indicate high nestedness or turnover, respectively,

There are serious problems with new indices, and consequently the literature on beta-diversity indices is complex and confusing. To provide an example, Baselga (2010) defines perfect nestedness as a spatial pattern where all species of the species-poorer assemblage are included in the richer assemblage so that the poorer assemblage has no

unique species. This definition agrees with the original definition of nestedness by Patterson & Atmar (1986) and with the definition of nested sets in mathematics, but, not with many of the indices proposed to measure nestedness, including Baselga's β_{nes}. We illustrate this by plotting β_{nes} against increasing species richness overlap of two assemblages (Fig. 1a). In Figure 1, the maximum $\beta_{nes} \cong 0.214$ is reached where 10 and 40 species are unique for the two assemblages (case D in Fig. 1a), which contradicts the conceptual definition. In addition, $\beta_{nes} \cong 0.1$ is attributed to three very different arrangements of species lists (Fig. 1) where: (i) 10 and 48 species are unique and two species are common to the assemblages; (ii) 10 and 22 species are unique and 28 species are common, and (iii) 10 and zero species are unique and 50 species are common. Apparently, the last arrangement is completely nested according to the conceptual definition and it should have the maximum value of β_{nes} (last case C in Fig. 1b). As different arrangements have equal values of β_{nes}, and maximum β_{nes} does not correspond to perfectly nested assemblages, the interpretation of β_{nes} as a metric of nestedness is invalid. We have therefore relabeled β_{nes} to β_{Bas} in our framework.

Here we offer an alternative framework for incidence-based indices measuring the (dis)similarity between two assemblages. We learn from the ideas and pitfalls spread across the literature (Simpson, 1943; Brualdi & Anderson, 1999; Lennon *et al*., 2001; Koleff *et al*., 2003; Gaston *et al*., 2007; Ulrich & Gotelli, 2007; Baselga, 2010; Lyashevska & Farnsworth, 2012) and take inspiration in physics and basic linear algebra. We show that the indices are tools to capture phenomena observed during fieldwork or data processing, and that these phenomena are already mutually dependent by their very nature, which prevents us from finding statistically independent indices. We further claim that the interdependence between the phenomena suggests that no partitioning of existing indices can purify an index from the effects induced by other phenomena, in order to better approach the focal phenomenon – for instance, species spatial turnover is affected by the difference in species richness, and removing this effect statistically does not lead to a proper inference, since the phenomena themselves affect each other. Therefore, instead of statistical independence of indices we advocate the independence of the indices in terms of the information they provide, adopting a *mathematical* concept of dependence. We develop guidelines to attribute the indices to different spatial phenomena. Finally, we demonstrate that a dependence between assemblages introduces interdependence between otherwise mutually independent indices, and that this effect sometimes obscures differences between otherwise clearly distinguishable patterns. Our framework addresses most of the problems that have repeatedly acted as incentives for generating new indices. In doing so, we demonstrate that most of the work needed has already been achieved by Jaccard (1912), Simpson (1943) and others in early 20th century (see also Tjørve *et al*., 2018).

Theory

This section is organized into several parts. Firstly, we describe five different spatial phenomena distinguished by ecologists, and show that these phenomena are different aspects of the structuring of biological diversity, which thus should be quantified by different indices. Secondly, we define the constraints necessary to attribute each of the indices to one spatial phenomenon. We argue that indices (mathematical expressions) should capture the intuitive understanding of their respective phenomena. Thirdly, we define the independence of biodiversity indices in terms of their information value. We show that we have to combine three indices that are independent in terms of their informational value, in order to make the correct and complete inferences about spatial and

temporal variation in biodiversity patterns. We contrast this independence with the independence that is often taken as a requirement for theories throughout ecological literature, defined as the absence of statistical correlation (Simpson, 1943; Koleff & Gaston, 2002; Jost, 2007). We show that the later independence is in most cases not obtainable and would not guarantee correct inferences about the spatial biodiversity pattern.

Distinguishing different spatial phenomena

Most diversity indices have not been defined *ad hoc*, but were deeply rooted in field experience, reflecting distinct spatial phenomena. Only the β_{gl} (Table 1) that measures species-richness gradient (Lennon *et al*., 2001), and the β_{Bas} (Table 1) seem to have originated from analyses of other indices and their interrelationships, i.e., from insights into the relationships between already invented indices. Three steps typically lead to an index definition: (i) field or data experience of a phenomenon; (ii) a discussion of the feature that captures the experience, and (iii) a mathematical formula or an algorithm that produces a one-variable proxy for the required feature. The one-variable proxy then becomes an index that is considered to capture the phenomenon. In the first two steps of the process, an ecologist formulates a predefinition of the observed phenomenon. These predefinitions are necessarily equivocal, allowing for more than one equation or algorithm that defines the index, but they allow for the exclusion of many mathematical formulas and algorithms from a list of candidates.

We propose that most of the commonly used indices have originated as proxies for *five spatial phenomena of ecology*: (1) Nestedness, (2) co-occurrence, (3) beta-diversity, (4) spatial turnover, and (5) species-richness gradient. Imagine ecologists roaming the landscape, leaving one site and approaching another. They would see changes in species richness, changes in species composition, and overlap in species composition between species assemblages. These correspond, in the same order, to several different (but not mutually exclusive) *patterns*, where: (i) species of the species-poor site are all present in the species-rich site; (ii) some species often co-occur at the same site, (iii) the checklist of species grows rapidly or slowly with increasing number of observed sites, (iv) new species replace the species of the site that the ecologist has left, but the species richness may or may not change, and (v) species richness either differs or remains the same between sites. Items (i-v) correspond to phenomena (1-5). A roaming ecologist would observe a combination of these patterns, as there are species-poor sites that host species missing in species-rich sites, and equally rich sites do not necessarily share the same set of species. Nevertheless, these five extreme patterns delimit the whole range of possibilities. So, the ecologist can intuitively classify assemblages in the field even without the knowledge of the mathematically defined indices. This is like comparing temperature, speed, or mass without measuring them.

<u>Nestedness:</u> The idea of nestedness was originally intended to capture the patterns in assemblages of archipelagos and/or of inland islands (e.g., mountain ridges). Patterson (1984), and Patterson & Atmar (1986) noticed that lists of species on mountain ridges varied, pointing at the situation where the species of the species-poor sites were almost universally found at the species-rich sites. They suggested that this pattern was driven by selective extinction and called it a nested pattern. Their index of nestedness, N_0, was designed to measure the deviation from a perfectly nested assemblage (where species-poor sites have no unique species). This concept of nestedness fully agrees with the mathematical definition of nestedness where a subset is nested within the set. Although the

original indices of nestedness (N_0, N_c, and Discrepancy, Patterson & Atmar, 1986; Wright & Reeves, 1992 and Brualdi & Sanderson, 1999) were designed for multisite assemblages, here we will explore them using only two assemblages (Koleff *et. al*., 2003; Gaston *et. al*., 2007), provided that the indices for multi-site assemblages are extensions of two-site indices.

Co-occurrence: Co-occurrence has been originally tightly linked with the idea that competition structures communities (Connor & Simberloff, 1979; Diamond & Gilpin, 1982), and with assembly rules (Diamond, 1975; Gotelli & McCabe, 2002). Species co-occur if their spatial ranges (distributions) overlap (Gotelli, 2000). If a species occurs at several sites, and another species occurs at only one of the sites, co-occurrence of these two is apparently low, although their ranges are nested within each other. This is the main difference between co-occurrence and nestedness. In the literature, however, co-occurrence typically refers to the overlap of species ranges and nestedness mostly refers to the overlap in assemblages. A closer look at several measures of nestedness, however, reveals that indices of nestedness are often used to indicate the overlap of species ranges (Wright & Reeves, 1992; Brualdi & Sanderson, 1999; Šizling *et al*., 2009), which makes nestedness and co-occurrence seemingly inseparable from each other. Here, we argue that nestedness and co-occurrence may both refer to overlaps in species ranges and assemblages, but that they differ from each other where overlap is small due to a large contrast between range areas or species richness. Then nestedness may be high, but co-occurrence low.

β-diversity: The original idea behind β-diversity is that different regions have different relationship between local (alpha) and regional (gamma) diversity. Beta-diversity thus quantifies the contrast between average alpha-diversity and gamma-diversity (Whittaker, 1960). Several authors offer different mathematical definitions of this contrast, but all of them assume that the region with the highest beta-diversity has the largest contrast between local and regional diversities, whereas the region with the lowest beta-diversity shows little contrast between local and regional diversities. Beta-diversity does not primarily compare two assemblages with different locations, but instead a set of sub-assemblages with a merged assemblage of the whole region. Although the Whittaker (1960) formula that defines beta-diversity was later included in the indices of similarity between two different assemblages (Koleff *et al*., 2003), we resonate with Koleff *et al*. (2003), Jost (2007) and Tuomisto (2010) that the two forms of comparison (i.e., between species richness of an assemblage and its sub-assemblages, and between two separate assemblages) should not be confused. This is so regardless of the known mathematical link between Whittaker beta and the Jaccard index of community similarity between adjacent plots (Tuomisto, 2010). The rationale is that mathematically similar equations do not always constitute equality between phenomena, and Whittaker beta and Jaccard index are interlinked only at the level of equations not at the level of phenomena. Separation of these two indices therefore helps us to draw unambiguous conclusions. Here we follow a similar logic as applied in physics, where 'work' and 'torque' are both computed as a product of force (F) and distance (r or d) ($W = F \cdot d$ and $\tau = F \cdot r$, in scalar form) and have equal units ($\mathrm{N} \cdot \mathrm{m}$), but differ in the direction of the acting force and should not thus be confused.

Species spatial turnover and species-richness gradient: Species spatial turnover explicitly addresses the gain and the loss of species in space (Cody, 1975; Wilson & Shmida, 1984). This covers a change in species richness (Harrison *et al*., 1992) and a change in species composition (Cody, 1975; Lennon *et al*., 2001). Although these two changes are bound by each other (change in species richness is always accompanied by a change in species composition to some extent), they are also mutually independent to some extent

(two equally species-rich assemblages can have all or no species in common). It is therefore useful to split turnover, in its broad sense, into these two components (Lennon *et al.*, 2001). Here we adapt the idea that the contrast between the species richness of two different assemblages (called species-richness gradient) and species spatial turnover are two different spatial phenomena (Lennon *et al.*, 2001).

These conceptual predefinitions are already mutually interconnected. Apparently, where no species co-occur there the turnover is higher than where all species co-occur. Where all species co-occur there all sites are occupied by equal set of species, and so there is no richness gradient and no turnover. Removing species from species poor assemblages increases both the richness gradient and turnover, and perfectly nested assemblages show smaller turnover than non-overlapping assemblages of the same richness. The interdependence of the phenomena is their inevitable property, which is necessarily reflected by any index.

Constraints needed to specify the phenomena

Next, we will develop a set of strict constraints that delimit the extreme cases of the phenomena described above. This will serve to attribute each index to a particular phenomenon. The simple way to describe the constraints mathematically involves six extreme re-arrangements of two sets as illustrated in the Venn diagram in Fig. 2. Each *set* can be considered either as a list of species or a species range. This allows us to identify the constraint of each phenomenon as imposed by its maximum value and its minimum value, and by ranking the situations that represent intermediate values. Below we show how individual phenomena have to be constrained to build meaningful indices.

- *Nestedness* has its maximum either where all the species from the species-poor list are found in the species-rich list (e.g., Patterson & Atmar, 1986; Baselga, 2010; Šizling *et al.*, 2016), or where one range falls completely within the second range for all species in the assemblage (e.g., Wright & Reeves, 1992; Brualdi & Sanderson, 1999; Šizling *et al.*, 2009). Therefore, two assemblages or ranges are maximally nested if one of them is completely contained within the other regardless of their size (as in re-arrangements r1,r2,r5,r6 in Fig. 2). The nestedness is at its minimum when none of the species is shared between two lists, or when there is no range overlap between two species (r3 and r4 in Fig. 2). No index should oscillate widely if an re-arrangement changes only slightly, which is the requirement of continuity *sensu* Neumann & Morgenstern (1953). Therefore, two *nearly* identical lists of species or two *nearly* identical ranges (r6 in Fig. 2) should have nestedness *near* to that of two *strictly* identical lists of species or ranges (r5 in Fig. 2). Since in the case of strictly identical lists one set of species is completely comprised within the other set, it also constitutes the maximum possible nestedness. This understanding is supported not only by the mathematical usage of the term "nestedness", which refers to a superset and its subsets, but it is also the basis of the conceptual (pre)definition by Patterson and Atmar (1986) and Baselga (2010). Therefore, we do not attribute zero nestedness to two equally rich assemblages or equally large ranges as did the inventors of N_0 (Patterson & Atmar, 1986), N_{NODH} (Almeida-Neto *et al.*, 2008), and β_{Bas} (Baselga, 2010). These and other indices that are automatically zero where species richness of the two assemblages is eqal ($S_X = S_Y$) do not discriminate between assemblages/ranges of equal size and zero overlap (r4 in Fig. 2) on one hand, and equal size and no (or partial) overlap on other hand (r5 in Fig. 2). This ambivalence would render the inferences from such an index of nestedness spurious.

- Maximum *co-occurrence* is where two species occupy the same sites (r5 Fig. 2), whereas minimum co-occurrence is where the ranges are completely non-overlapping (r3, r4 in Fig. 2). Species that share only part of their ranges (r1, r2, r6 in Fig. 2) co-occur less than species with identical ranges (r5 in Fig. 2) and more than species with no shared occurrences (r3,r4 in Fig. 2). The distinction between nestedness and co-occurrence therefore lies in re-arrangements r1 and r2 (Fig. 2), with equal nestedness ($\mathrm{Nest}[r1] = \mathrm{Nest}[r2]$ in Fig. 2) but different co-occurrence ($\mathrm{Co}[r1] < \mathrm{Co}[r2]$ in Fig. 2). We hold that species whose ranges are perfectly nested, but differ in their size, have a lower co-occurrence than species with two identical ranges ($\mathrm{Co}[r2] < \mathrm{Co}[r5]$ in Fig. 2).
- *Beta-diversity*, as it is understood here, does not capture the similarity between two assemblages, but rather the contrast in species richness between two scales (between a region and a sub-region, or between a total area and a sample unit). It is therefore logical that the β-diversity of the set illustrated by r1 in Fig. 2 is higher than that of r2 in Fig. 2, if M4 and M5 are sub-assemblages of M1 and M3, respectively. Similarly, the beta-diversities in r5 and r6 Fig. 2 are none and almost none, respectively.
- *Turnover* captures the contrast in species composition between two or more assemblages. Consequently, the turnover found in re-arrangement r3 in Fig. 2 must be larger than that of r1 in Fig. 2, which in turn represents a larger turnover than r2 in Fig. 2. In r5 Fig. 2, the species lists or ranges are identical hence there is no turnover at all, which means that the index of turnover is at its minimum. However, it is not intuitively evident whether the case r3 represents a larger turnover than that of r4 in Fig. 2. In our framework, we distinguish between turnover and species richness gradient (SRG, Lennon *et al.*, 2001) and so we solve this dilemma by stating arbitrarily that $\mathrm{Turn}[\mathrm{r3}] = \mathrm{Turn}[\mathrm{r4}]$ but $\mathrm{SRG}[r3] > \mathrm{SRG}[r4]$ (Fig. 2).
- Because we define the *species-richness gradient* (SRG) as simply the contrast in species richness between two sites, the re-arrangements r1 and r3 in Fig. 2 represent the same SRG, as do r4 and r5 in Fig. 2. The latter also represents a zero SRG and therefore the minimum. Consequently, the value of the SRG in r2 Fig. 2 falls between the above.

Importantly, the constraints do not define the indices uniquely and two different indices (i-independent in the sense of the forthcoming section) may obey the same constraints. In this case we say that these two indices capture two different aspects of the same spatial phenomenon.

Independence in terms of information content

To capture different spatial phenomena by different indices, we need an idea of an independence of indices in terms of their information content – only the indices that do not carry the same information can distinguish different phenomena. To find out the information provided by an index, we need to see the definitions of the indices as equations to solve (Box. 1). When we add an equation to the set of *n* equations, and if these *n*+1 equations provide equal solution as the set of n equations, then the new equation is said to be dependent on the others and carries no extra information. If the solution of the *n*+1 equations is a subset of (but not equal to) the solution of the *n* equations, then the new equation is independent of the others and carries extra information. Note that this is the mathematical definition of independence (see also Box 1). In extreme circumstances, the set of equations with one unique solution carries complete information on assemblages to interpret. In the case of two assemblages, it all means that the complete set of equations

uniquely determines richness of both assemblages (S_X, S_Y) as well as species overlap ($S_{X\cap Y}$; for details see Box 1).

We extend the mathematical definition of independent equations, and define the indices that are mutually independent if the equations of the indices are mutually independent (Box 1). The β'_{Sim} (one minus Simpson beta) and J (Jaccard similarity) (Table 1) are mutually independent because there is no way to compute β'_{Sim} from J. This is easy to see from Fig. 3a and b, where more than one value of β'_{Sim} is attributed to each value of J ($J \neq 0$). This is an analogy to a case from physics, where the kinetic energy (E_k) and momentum (p) of a moving object cannot be calculated from each other although they are computed using the same variables ($E_k = 0.5mv^2$, $p = mv$; m is mass and v is speed). It induces mutual, but *not one-to-one* correspondence (Fig. 4) between energy and momentum (Fig. 3c, d). However, because E_k and p are independent in terms of the lack of *one-to-one* correspondence, the equations of these variables can be combined to determine the mass and speed of an object. All this means that J and β'_{Sim} carry different information about assemblages, similarly to E_k and p which carry different information about moving objects, although statistical tests would reveal their mutual statistical dependence.

In contrast to this definition of independence, the independence that is used in ecological literature is almost always of statistical nature. This is different from the independence between indices in terms of their informative value, as explained above. For simplicity, we hereafter refer to the former mathematical independence as *i-independence*, which stands for *informational* independence, and the latter as *s-independence*, which stands for *statistical* independence. While the i-independence refers to a mathematical formula, the s-independence refers to data values (i.e., a conditional probability of measuring a particular value of one variable, given a value of another variable).

Some indices are i-independent, while their values are s-dependent. For example, J and β'_{Sim} are i-independent, but their values generated across all possible assemblages are s-dependent (Fig. 3a, b).

Forces that drive statistical dependence

S-dependence of indices is driven by bounds that the indices impose upon each other. For example, J and β_{Sim} are bounded by each other, because $S_X + S_Y$ is always larger or equal to twice $\min(S_X, S_Y)$. From combining the definitions of J and β'_{Sim} (Table 1) it follows that

$$\beta'_{Sim} = \left(\frac{S_X+S_Y}{\min(S_X,S_Y)}\right)\left(\frac{J}{1+J}\right) \geq 2\,\frac{J}{1+J} \qquad (1)$$

(SI.3.T3). This bound on β'_{Sim} (the inequality) imposes s-dependence between J and β'_{Sim}. A limit on one index by the second index can be obtained for any two i-independent indices that are computed using S_X , S_Y, and $S_{X\cap Y}$ and are i-independent of total species richness (Box. 1). The point is that the more variables that are shared between definitions of two indices, the more links are between them. This is the mathematical reason for the interdependence between the phenomena and the reason why indices are likely s-dependent regardless of their i-independence (Lyashevska & Farnsworth, 2012).

The Jaccard index, and thus all the indices that scale in a one-to-one manner with the Jaccard index (i.e. there is a bijection between them, Fig. 4) has been referred to as 'dependent' on species richness of the assemblages (Simpson, 1943; Lennon *et al*., 2001; Koleff & Gaston, 2002; Baselga, 2010). This has led to a search for an index that is species richness 'independent' or an attempt to modify the Jaccard index, which was motivated by a

need to compare assemblages of two regions or two time periods that varied in species richness. The reported 'dependence' between the Jaccard index and species richness was based on empirical experience (Koleff & Gaston, 2002), or on arguments that there are bounds on the Jaccard index imposed by the species richness (Simpson, 1943). Hence, this kind of dependence is a statistical one. In terms of information, the Jaccard index is i-independent of species richness. The reason is that *J* satisfies the equation

$$\frac{\rho \cdot S_{X\cap Y}}{\rho \cdot S_X + \rho \cdot S_Y - \rho \cdot S_{X\cap Y}} = \frac{S_{X\cap Y}}{S_X + S_Y - S_{X\cap Y}} = J, \quad (\rho \neq 0) \tag{2}$$

and thus it does not change when S_X, S_Y, and $S_{X\cap Y}$ scale in the same manner. In this case, the Jaccard index returns the same value regardless of the species-richness, and thus species richness does not uniquely determine *J* (see SI.3.T1 for more formal proof using Cramer's rule). Any observed s-dependence between the Jaccard index and species richness is therefore caused by disproportional scaling in S_X, S_Y or $S_{X\cap Y}$. This holds true for all the indices under discussion (Cody, 1975; Weiher & Boylen, 1994; Gaston *et al*., 2007).

The Jaccard index is not bounded by total species richness, since species richness affects neither the upper nor the bottom limit of the Jaccard index. The evidence is that we can re-organize species in assemblages of any species richness (which is kept constant for different re-organizations) to get *J*=0 or *J*=1. It makes $S_{X\cap Y} = 0$ and S_X, S_Y unlimited for $J = 0$, and $S_{X\cap Y} = S_Y = S_X$ for $J = 1$, where S_X is again unlimited. However, the frequency distribution of possible Jaccard values is affected by total species richness. This in turn affects the most likely value of the Jaccard index, imposing its s-dependence on species richness. The reason is that the Jaccard index can only return a restricted number of values. For example, if $S_X = 1$ then $J = 1, 1/2, 1/3, 1/4, \ldots, 0$, accumulating possible values below 1/2. $S_X = 2$ then allows for 2/3, which is above 1/2, $S_X = 3$ allows for $3/4 > 2/3$ and so on. Further computation of possible *J* values for increasing S_X (Fig. SI.4) shows a progressively more even distribution of *J*-values.

The bounds on the Jaccard index are thus not given by species richness itself but by the interplay between the larger value of S_X and S_Y, and by the difference between them. The reason is that the value of J is by definition never larger than the ratio of maximum possible $S_{X\cap Y}$ to minimum possible S_{TOT} ($= S_X + S_Y - S_{X\cap Y}$). This extreme re-arrangement emerges when the smaller assemblage is perfectly nested within the larger assemblage. Considering that $S_{X\cap Y} \leq \min(S_X, S_Y)$ and $S_{TOT} \geq \max(S_X, S_Y)$, then

$$J \leq \frac{\min(S_X, S_y)}{\max(S_X, S_y)} = 1 - \frac{|\Delta S_{XY}|}{\max(S_X, S_y)} \tag{3}$$

where $|\Delta S_{XY}|$ is absolute value of the difference between S_X and S_y. It follows from Eq. 3 that the upper limit of J increases with decreasing $|\Delta S_{XY}|$ and increasing $\max(S_X, S_y)$. That is, the lower the maximum species richness and the larger the difference between species richnesses, the smaller is the expected J. This reasoning extends and formalizes the point made by Simpson (1943) who identified $|\Delta S_{XY}|$ to bound J, and Koleff *et al*. (2003) who discussed the s-dependence of *J* on species richness. These bounds, however, do not induce an inevitable correlation in observed data. In real data, there may be other (biological) reasons for the correlations between indices, which may go against the statistical effect of the bounds discussed here.

Statistical correlations are thus expected even among i-independent indices due to the bounds they impose on each other. However, since these bounds follow from the very nature of studied phenomena, attempts to remove these effects lead necessarily to indices that measure something that is only loosely linked to the phenomena.

Results

Families of indices

So far, we have developed theory to assign indices to different phenomena. Mathematically, however, it is more feasible to first group the existing indices into families with equal information which thus capture the same phenomena. We can then proceed by assigning a phenomenon to one index from the respective family which is most often used or most convenient for some reason (one can then always recalculate all the indices to another index, Box 2). We have done this in appendix SI.3.T1-19, and here we summarize the results.

There is a number of diversity indices and each has some information value. Some of them, however, are i-dependent, and they are equivalent in terms of any inference. To distinguish families of equivalent indices, we first examined the mutual scaling of indices. The mathematically correct and accepted way to do this was to plot the indices against each other, using simulated and empirical data (Figs. 5-7). Where we did not see a one-to-one correspondence (Fig. 4), i.e. the line joining the points in the plot was neither strictly increasing nor strictly decreasing, the two plotted indices were considered mutually i-independent. Where we saw a one-to-one correspondence along a strictly increasing or decreasing curve, we had to prove the i-dependence by mathematical analysis. This way we found two big and five small families of mutually equivalent indices (Fig. 5), and the mathematical analysis (SI.3) confirmed the one-to-one correspondences between the indices within these families. These families are:

1. Jaccard index family. The largest family of indices is grouped around the Jaccard index (Jaccard, 1912). It has 9 indices of (dis)similarlity, including Sørensen ($\beta_{Sør}$, as defined in Gaston *et al.*, 2007), β_{HK} (Harte & Kinzig, 1997), β_G (Gaston *et al.*, 2001), β_{SR} (Schluter & Ricklefs, 1993), β_t (Wilson & Shmida, 1984) and β_{DICE} (Raup & Crick, 1979). The Bray-Curtis index of dissimilarity (β_{BC}, Bray & Curtis, 1957), belongs to the Jaccard index family when computed from incidences. A classical index of nestedness, N_c (Wright & Reeves, 1992), is the number of cases where presence of a species at a species poorer site predicts its presence at the richer site, that is, $S_{X\cap Y}$ for the two sites. The N_c also belongs to the Jaccard-index family (Fig. 5, SI.3.T8) when standardized by $S_X + S_Y$ (Gotelli & McCabe, 2002). The indices of the Jaccard-index family capture the phenomenon of species turnover (Fig. 8, SI.3.T15). To be precise, J measures species co-occurrence (proportion of species that co-occur in both assemblages), which is a reversed measure of species turnover (the relationship between an index and the reversed index is strictly decreasing), and all indices from the Jaccard-index family that decrease with increasing J (e.g., β_t or $\beta_{Sør}$) are measures of turnover (Fig. 2). Jaccard index represents a type of similarity that scales inversely with turnover. This supports the point of Gaston *et al.* (2001) who defined an index of turnover, β_G, as

$$\beta_G \stackrel{\text{def}}{=} \frac{S_X+S_Y-2S_{X\cap Y}}{S_X+S_Y-S_{X\cap Y}} = 1 - J. \qquad (4)$$

Indices from Jaccard family are the only measures (or reversed measures) of co-ooccurrence of two species if we replace S_X, S_Y and $S_{X \cap Y}$ with numbers of occupied sites by species X and Y

2. Simpson-beta family. The second family consists of Simpson's beta (β_{Sim}, Simpson, 1943), r-Nestedness (rN, applied to species lists; Šizling *et al*., 2009), and Simpson's nestedness (β'_{Sim}, Šizling *et al*., 2016). As β'_{Sim} is identical to rN when applied to species lists, we do not plot these indices separately in Fig. 2. Two classical indices of nestedness, the Discrepancy (D, Brualdi & Sanderson, 1999), and the standardized N_C by Wright & Reeves (1992) also belong to the Simpson-beta family under certain circumstances. Specifically, D follows β_{Sim} if computed for multisite assemblage and the number of sites is high enough (SI.3.T13). D (standardized as in Greve *et al*., 2005) converges to the mean across all β_{Sim} (i.e. $\langle \beta_{Sim} \rangle$) as number of sites increases. In practice, n>10 guarantees

$$D \cong \langle \beta_{Sim} \rangle \qquad (5)$$

(Fig. SI.5). N_C belongs to Simpson beta family if standardized as suggested by its authors (Wright & Reeves, 1992) and if species richness is high (SI.3.T9). The indices from the Simpson-beta family capture the phenomenon of nestedness (SI.3.T4). β_{Sim} and D are measures of reversed nestedness, whereas β'_{Sim} and rN measure the nestedness applied at the level of assemblages and ranges, respectively.

The third to sixth families are each made up of only a single index. Neither of these indices capture any phenomenon under consideration (SI.3.T7,10,12). These are:

3. Ruggiero index of beta-diversity (β_{Rib}, Ruggiero *et al*., 1998). β_{Rib} is defined in a similar manner to the β_{Sim}. However, the β_{Rib} measures geographic asymmetry, whereas the β_{Sim} is a symmetric index. This means that β_{Rib} changes when assemblages are relabelled (S_X is replaced with S_Y and S_Y with S_X), while the β_{Sim} is robust against such relabelling. This is because the β_{Sim} is normalized by the species-poorer assemblage, and the β_{Rib} is normalized by the assemblage that we are approaching. β_{Rib} therefore equals the β_{Sim} in all cases where we are going from species-rich to species-poor assemblages. One could say that the β_{Rib} measures how much the approached assemblage is nested within the assemblage that we are leaving. The β_{Sim}, on the other hand, is a measure of the extent to which the species-poorer assemblage is nested within the species-richer assemblage. The β_{Rib} thus belongs to the Simpson-beta family only under certain circumstances and can be considred neither fully i-independent nor fully i-dependent on the β_{Sim} .

4. Baselga nestedness component of beta-diversity (β_{Bas}, labelled as β_{nes} in Baselga, 2010).

5. The classic index of nestedness, N_0, (computed for two sites; Patterson & Atmar, 1986).

6. The N_{NODF} index of nestedness (computed for two sites; Almeida-Neto *et al*., 2008). The N_{NODF} would have belonged to the Simpson-beta family if it had not been automatically zero for $S_X = S_Y$, regardless of $S_{X \cap Y}$ (SI.3.T12). This condition splits the scaling line in the bivariate plot into two different trajectories (Fig. 2), which makes any inference difficult in the same way that we have demonstrated for β_{Bas} in the Introduction section.

*7. Species richness gradient***.** The index that is central to the seventh family is β_{gl}, (Table 1, Lennon *et al*., 2001). The β_{gl} captures the contrast in species richness between two sites, which is the phenomenon of species richness gradient (SI.3.T14). In addition to β_{gl} we propose a new index for this family:

$$R \stackrel{\text{def}}{=} \frac{\min(S_X,S_Y)}{\max(S_X,S_Y)} =_1 \frac{2-\beta_{gl}}{2+\beta_{gl}} =_2 \frac{J}{J(\beta'_{Sim}-1)+\beta'_{Sim}}, \qquad (6)$$

and we name it index of species richness uniformity. The first part ($=_1$) is derived in SI.3.T19, and the second ($=_2$) follows from Eq. B5 (Box. 1). The rationale is that the index value (R) approaches 1 where there is no spatial variation in species richness, and 0 where species richness varies considerably. R is simpler than β_{gl}, and it also simplifies the mathematical formulae for the relationships between the families (Eqs. 7-12).

i-independent combinations of indices

Although we have delineated eight families of indices, it does not mean that there are eight i-independent indices. The reason is that three indices from any three families are i-dependent even if any single pair from this triplet is i-independent. Only two families are then i-independent with certainty, and the indices of the other families can be determined from these two (Box 1). A clear case of mutual i-dependence of a triplet of indices is the combination of the Jaccard-index family, the Simpson-beta family and the species-richness-gradient family. A simple rearrangement of Eq. 6 gives

$$\frac{J}{1+J} = \beta'_{Sim}\,\frac{R}{1+R}, \qquad (7)$$

which says that reversed turnover) increases with increasing nestedness and species richness uniformity (reversed gradient) in a multiplicative manner. The result (Eq. 7) can be generalized to all the considered indices listed in SI.2 (Box. 1).

We can also extend our considerations to multisite assemblages. From Eq. 7 it follows (see SI.3.T19 for derivation, and Fig. SI.6 for data-based evidence) that

$$\langle\frac{J}{1+J}\rangle = \langle\beta'_{Sim}\rangle\,\langle\frac{R}{1+R}\rangle + cov(\beta'_{Sim},\frac{R}{1+R}) \cong (1-D)\,\langle\frac{R}{1+R}\rangle, \qquad (8)$$

where the brackets ⟨ ⟩ label a simple mean across all values of the expression between them (if *J*=0.1, and 0.2, then $\langle J/(1+J)\rangle \cong 0.129$). The first equality is a simple consequence of the definition of covariance, and the second (approximate) equality results from Eq. 5 and the assumption that the covariance is negligible. Negligible covariance is likely, because the phenomena of nestedness and species-richness gradient do not constrain each other, and therefore the β'_{Sim} and $R/(1+R)$ are s-independent (SI.3.T19), unless there is an ecological mechanism forcing the covariance away from zero (Fig. SI.6). Therefore, mean pairwise indices can characterize multi-site assemblages, and the interrelationships of mean pairwise indices hold under some (realistic) circumstances. The mean pairwise values (i.e. the means in Eq. 8) have been criticized for inaccuracy that results from employing each value several times in an index calculation or in statistical tests (e.g., Sokal, 1979; Legendre *et al*., 2015), but this only affects variance, not the means. Mean values cannot be affected by using the values more than once providing that each value is equally employed.

Special cases: families of indices when assemblages are spatially autocorrelated

The mutual i-independence of the indices implicitly assumes that species assemblages are completely 'independent' of each other, and that spatial proximity of the assemblages or

similarity between habitats do not affect i-independence between the indices. However, this may not be the case, as assemblages are often spatially auto-correlated due to similarity in habitats or mass/rescue effects (Brown & Kordic-Brown, 1977). This leads to two special cases of behavior of the indices. First, let us assume some effects that limits species richness variation between sites. In extreme, $S_X = S_Y$. In this case, there is no sr-gradient, $R = 1$ and Eqs. 7 and 8 turn into

$$\beta'_{Sim} = 2\frac{J}{1+J} \text{ and } \langle\beta'_{Sim}\rangle = 2\langle\frac{J}{1+J}\rangle. \quad (9)$$

This means that the Jaccard-index and the Simpson-beta families become i-dependent (Fig. 6a). Second, autocorrelation can cause assemblages to be perfectly nested, i.e. the species-poor assemblages have no unique species. In this case, $S_{X\cap Y} = \min(S_X, S_Y)$ and so $\beta'_{Sim} = 1$. It follows from Eqs. 7 and 8 that

$$\frac{J}{1+J} = \frac{R}{1+R} \Longrightarrow J = R, \text{ and } \langle\frac{J}{1+J}\rangle = \langle\frac{R}{1+R}\rangle. \quad (10)$$

It reads that the Jaccard-index and the sr-gradient families are no longer i-independent (Fig. 6b). These special cases can easily be recognized in any data. It follows that $\langle\beta'_{Sim}\rangle$ approaches one in the case of a fully nested pattern, and $\langle 2J/(1+J)\rangle$ (see Eq. 9) in the case of a low spatial variation in species richness. In the latter case $\langle R\rangle$ approaches one.

The loss of i-independences in these special cases is trivial, but it illustrates an important point: Even if indices are i-independent, they appear more dependent on each other as species richness values across sites become similar, and/or when the assemblages approach complete nestedness (compare Figs. 5 and 7).

Statistical equivalency of the indices

We have argued that the indices within a given family are equivalent – since they are i-dependent and provide the same information. However, they are not equivalent statistically. The reason is that they often scale non-linearly with each other. For instance, within the Jaccard-index family there are three groups of indices that scale in a linear manner (group i: J, β_G; group ii: N_c, t, β_{sr}, β_{HK}, β_{BC}, $\beta_{Sør}$; group iii: β_{DICE}; Fig. 2), and are statistically equivalent. Between these groups, however, the indices scale nonlinearly (see, e.g., J and β_{Sor} in Fig. 5), and this decreases the correlation coefficient between otherwise i-dependent indices, which decreases s-dependence between the indices (e.g., Koleff & Gaston, 2002; Lyashevska & Farnsworth, 2012).

The values of an index within one family that scales in a non-linear manner (Fig. 4) with another index can also be seen as transformed values of the other index. For example, the $\beta_{Sør}$ and β_{HK} are two indices that originated as equal transformations of J (Fig. 5, SI.2). However, this means that these values have different frequency distributions, which can affect statistical tests and their sensitivity. This could lead to the conclusion that it is always necessary to use one index which is most symmetric/regularly distributed for given system. However, the existing and commonly used indices represent a rather poor spectrum of transformations (Fig. 5). It would be thus more practical to adapt various transformations of the indices (e.g., logit) that are central to the families than pick and choose from the range of existing indices. Alternatively, it is possible to test the index values against a null model, and then the distribution of the values is not an issue (Ulrich & Gotelli, 2007, 2013; Chase *et al.*, 2011).

Making inference out of the indices

We have shown that it makes little sense to develop indices that purify one aspect of diversity patterns, controlling for the other aspects; an example is the futile attempt to partition the nestedness and turnover components sensu Baselga (2010). The reason is that s-dependence represents an inherent property of the phenomena, where different aspects bound each other. Inequality in species richness (diversity gradient) bounds possible values of species turnover, imposing its bottom limit, to provide an example. An effort to remove one aspect from the overall pattern thus leads to spurious results and misleading interpretations.

Inference from the indices can have different purposes (Anderson *et al.*, 2010): (i) exploration of the (dis)similarity between biotas of two regions (e.g., Simpson, 1943), (ii) comparison of spatial diversity patterns between regions (e.g., Qian *et al.*, 2009), (iii) revealing non-random origin of a spatial or temporal biodiversity pattern (e.g. Patterson & Atmar, 1986), (iv) meta-analysis based on indices extracted from the literature, and (v) exploration of the behavior of the indices along a temporal, spatial or environmental gradients (e.g. Storch *et al.*, 2005). In all situations when we compare two regions or periods, or test for (non)randomness in spatial diversity pattern with respect to a particular phenomenon, a single index is sufficient regardless of its s-dependence on other indices. We will demonstrate the irrelevance of s-dependence of indices on the triplet J, β'_{Sim}, R, as all presence-absence indices of (dis)similarity between two assemblages are convertible to two of these three indices (Box. 2). S-dependence between these indices is driven by inequalities:

$$0 \leq J =_1 R\frac{\beta'_{Sim}}{R+1-R\beta'_{Sim}} \leq_2 \frac{\beta'_{Sim}}{2-\beta'_{Sim}}, \text{ and } 0 \leq J \leq_3 R. \qquad (11)$$

The first equality ($=_1$) results from Eq. 7, the next inequality ($\leq_2$) involves β'_{Sim} and is a consequence of $0 \leq R \leq 1$, and the last inequality ($\leq_3$) is a consequence of $0 \leq \beta'_{Sim} \leq 1$ and the first equality ($=_1$). Both bounds ($\leq_{2,3}$) have been taken as an argument that J and β_{Sim} have to be corrected for the effect of the other indices (e.g., Simpson, 1943; Baselga, 2010). We argue that (i) the Jaccard index is a measure for reversed turnover or co-occurrence regardless of the bounds, and that (ii) the bounds only show the limits of maximum possible reversed turnover given the level of nestedness or uniformity (*R*) in species richness across sites. The value of the Jaccard index relative to its maximum ($\leq_1$) shows the level of uniformity (Fig. 8). It is similar to an understanding that electric current cannot reach any value, but is limited by the resistance of the focal electric element and maximum possible voltage of the source.

In all situations when only the index values are available (e.g., raw presence/absence data are missing, because the indices are extracted either from the literature or from incomplete data), we have to combine information from more indices for the full inference (Table 2). Although all the information is stored in *J*, β'_{Sim} and $\langle S \rangle$ (or other three i-independent indices) it is also useful to compute *R*, together with the contribution of species-poor and species-rich sites to the average alpha diversity. These contributions follow

$$S_{poor} = \langle S \rangle \frac{2R}{R+1}, S_{rich} = \langle S \rangle \frac{2}{1+R} \qquad (12)$$

and result from solution of Eqs. B3 and B4 (Box. 1, see SI.2.T17 for the derivation). Variation in S_{poor} and S_{rich} indicates the sites that contribute to the variation in J, β'_{Sim}, and R (Table 2).

To summarize, (i) if $\beta'_{Sim} = 0$, assemblages are non-nested, and J is automatically 0 regardless of the species richness gradient, carrying no extra information; but (ii) where $\beta'_{Sim} \neq 0$, β'_{Sim} measures the extent to which the species-poorer assemblages are nested within the species-richer assemblages, and J is then the similarity that is a reversed species spatial turnover. We need, however, to distinguish between the value of J, which measures reversed turnover per se, and J relative to its upper limit J_{max} (Eq. 11, Fig. 8), which scales inversely with species-richness gradient (R, or β_{gl}). Therefore, the combination of *J* and *R* is sufficient for any inference.

To provide a case study we use indices from Šizling *et al*. (2016) who studied temporal change of Central European plants during Holocene. They reported an increase in mean species richness $\langle S \rangle$ from 23 to 36, almost no change of β'_{Sim} ($\beta'_{Sim} \cong 0.7$), and an increase of average J from approximately 0.38 at the end of the last Ice Age to the recent value of approximately 0.48. Based on Eqs. 7 and 12, the R increased from 0.65 to 0.86, S_{poor} increased from app. 18 to 33, and S_{rich} increased from app. 28 to 39. Based on our framework, we conclude that recent plant assemblages in Central Europe show lower spatial turnover (higher similarity), and lower species-richness gradients than those about 14,000 years ago. Nestedness has not changed during this period, however, the contribution of species-poor sites to the mean alpha diversity increased more ($\Delta S_{poor} = 15$) than contribution of species rich sites ($\Delta S_{rich} = 11$). The spatial pattern in plant diversity therefore became more uniform with a proportionally higher increase of richness at species poor sites, and increasing average diversity of the sites. Regardless of the higher recent uniformity, the species poor sites used to have similar proportion of unique to common species as today.

The results of our analysis of the indices directly contradict Baselga's (2010) interpretation. When we used Baselga's (2010) partitioning method on our Holocene plant data, we got $\beta_{Bas} = 0.25$, $\beta_{Sim} = 0.3$ for the past and $\beta_{Bas} = 0.34$, $\beta_{Sim} = 0.3$ for the recent. This reads in the Baselga's (2010) framework as no temporal change of turnover and an increase of nestedness, which is the exact opposite to our results. Furthermore, Baselga's (2010) interpretation suggests stronger contribution of turnover than nestedness in the past ($\beta_{Bas} < \beta_{Sim}$), but the patterns reported above, based on direct interpretation of i-independent indices, do not suggest anything like that. We have demonstrated that nestedness and turnover are incomparable, thus it is impossible to say whether nestedness contributes to species pattern more or less than turnover. To exemplify this point, *J* is always smaller than β'_{Sim}, which might suggest a universally higher contribution of turnover than nestedness. But the square of β'_{Sim} is also a measure of nestedness and it is sometimes smaller than *J*, suggesting the opposite contribution (e.g., $\beta'^2_{Sim} \cong 0.07 < J \cong 0.1 < \beta'_{Sim} \cong 0.3$ for $S_X = 33$, $S_Y = 63$, $S_{X \cap Y} = 9$). This reasoning also applies to the Baselga (2010) framework. In the case of our Holocene plant data example, $\beta^2_{Sim} = 0.09 < \beta_{Bas} = 0.25 < 0.3 = \beta_{Sim}$ in the past. However, β_{Sim} and β^2_{Sim} mutually scale in one-to-one manner and thus must measure the same phenomenon. Hence, the the phenomena that are measured by β_{Sim} and β_{Bas} are incomparable. In conclusion, a comparison of the contributions of any two phenomena is meaningless, as no phenomenon has one 'true' measure.

Discussion

Problems with previous approaches

We have proposed a consistent framework for presence-absence biodiversity indices. We have identified the sources of the proliferation of new indices in ecological literature as: (1) the search for statistical-independence of indices, (2) the habit of designing indices without considering all constraints necessary for delineating the phenomena that the indices aim to capture, and (3) the lack of tools to make inferences about spatial and temporal bio-diversity patterns. We have designed our framework to avoid these pitfalls.

We demonstrated that it is pointless to search for s-independent indices, because (i) s-independence concerns index values instead of index formulae and thus s-dependence is a matter of the structure of data rather than index definitions; and (ii) s-dependent values emerge even from the desired i-independent indices. This is true regardless of the exact mathematical definition of an index because s-dependence follows from the links between conceptual pre-definitions of the phenomena. In other words, there are no s-independent indices that capture different, but necessarily mutually dependent phenomena. On the other hand, the dependence between the phenomena that induces the s-dependence of indices still allows the indices to be i-independent of each other. In the indices, the s-dependence is realized via S_X, S_Y, and $S_{X\cap Y}$, that are shared by the index formulae, and that constrain the indices. The s-dependence is thus a property of particular data, and should not bother us if we draw the inferences properly.

We revealed the limits of partitioning diversity indices into s-independent components in order to define new indices, as suggested by Baselga (2010) and Lennon *et al.* (2001). The idea behind the partitioning was that new indices that capture s-independent components of the phenomena could be created by combining the existing indices. A similar idea was also applied to indices based on abundances (Jost, 2007), but see Reeve at al. 2016 for partitioning abundance-based indices that conforms to our framework. However, we now know that while a new index should be i-independent of others, any combination of already existing indices only produces an i-dependent index. No partitioning of these indices can solve the problem of i-dependence, or purify the index to make it a better proxy for a focal phenomenon. The only proper way to partition an existing index is to first split the phenomenon (not the index) in terms of its conceptual pre-definition. A good example of this approach is presented by Lennon *et al*'s. (2001) who partitioned turnover into 'pure' turnover and species-richness gradient. The fact that Lennon *et al*. (2001) did not partition an index but the phenomenon is why we adopted the idea into our framework.

The reason why β_{Bas}, N_0, and N_{NODF} all fail to measure what was conceptually pre-defined as nestedness (e.g. by Patterson & Atmar, 1986) is that these indices have not been checked against a sufficiently wide range of constraints or extreme cases. This is best seen in Fig. 6. In Fig. 6b, all pairs of the assemblages are simulated as perfectly nested, but β_{Bas} and N_{NODF} have multiple values that disqualify them from identifying a nested biota. In Fig. 6a, none of β_{Bas}, N_0 or N_{NODF} varies despite the fact that the assemblages were simulated to show various levels of nestedness as defined conceptually. These indices therefore do not distinguish between perfectly nested and non-nested biotas. In particular, none of these three indices was anchored by constraints in r4 and r5, Fig. 2. On the other hand, the indices of the Simpson-beta family do identify perfectly nested biotas. This is supported by Fig. 6b which shows no variation in values of these indices across different absolutely nested

biotas, and Fig. 6a which show how values of these indices vary where biota is partially nested and partially non-nested (for precise evidence see SI.3).

Spatial diversity phenomena and classes of indices

We have shown that the five spatial phenomena of diversity are mutually dependent, with mathematical links between their indices. As a result, only two i-independent indices at a time (for example J and β'_{Sim}) are sufficient to provide information on nestedness, co-occurrence, turnover and species richness gradient. In addition, we need the index of Whitaker beta-diversity, whose link to other indices has not been exactly formulated. Whittaker beta-diversity is widely believed to be dependent on turnover, but the exact mathematical link has been revealed only for adjacent sub-regions that make together the whole region (Koleff *et al*., 2003; Tuomisto, 2010; Šizling *et al*., 2011).

We have replaced the need for s-independent indices with a need for i-independent indices. However, sufficient i-independent indices have already been invented, and there is thus no need for new indices, nor for their partitioning to achieve s-independence. This is because s-independence cannot be universally achieved. We have shown that two i-independent indices describe the system, so that in combination with a species richness value (which acts as a scaling parameter) they provide complete information of the system. However, one index is sufficient when the variation of species richness across sites is negligible, or when there are no species that are unique to the species-poorer assemblage (i.e. perfect nestedness). The problem is that species-richness uniformity or autocorrelation make some families almost indistinguishable (Fig. 7) and certain degree of autocorrelation is often found in natural assemblages (Simbleroff & Martin, 1991; Wright & Reeves, 1992; Cook & Quinn, 1995). It thus has been difficult to achieve agreement regarding which indices characterize different phenomena (Lennon *et al*., 2001; Gaston *et al*., 2007; Ulrich & Gotelli, 2007; Baselga, 2010; Tuomisto, 2010), given that the correlations between the observed index values are higher than what would follow from the theory alone.

Our findings have important consequences for understanding to the forces shaping distance decay in assemblage similarity (Nekola & White, 1999). A direct consequence of Eq. 7 is that distance decays of nestedness (β'_{Sim}) and turnover (measured by $J/(1+J)$) follow the same mathematical function only when there is no distance decay in the sr-gradient. This happens only in environments without geographical gradients that affect the species richness, for example, gradient in productivity (e.g., Willig *et al*., 2003; Currie *et al*., 2004). In these cases spatial structuring of the assemblages is anisotropic, and there are different rates of distance decay in different directions. Even more importantly, it is meaningless to assume a universal functional form of the distance decay of community similarity, e.g. exponential (Nekola & McGill, 2014). This follows from the mutual non-linear scaling between different indices, even between the i-dependent ones. Consequently, if one index reveals, say, exponential distance decay, another index can reveal a non-exponential distance decay.

In conclusion, our framework systematically deals with problems that unnecessarily generated new indices, and it resolves old issues concerning the mutual dependence of the indices. Based on the distinction between two types of dependence (i- vs s-dependence), we offer a tool for making inference using classical indices, a tool that can be further developed when new spatial or temporal phenomena are identified. Our framework is consistent as a whole, which is an advantage over earlier works that have accumulated new indices and phenomena without a unifying concept.

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Table 1: The frequently used pairwise indices. S_X and S_Y are Species Richness of the assemblages to compare , and $S_{X\cap Y}$ is the number of shared species between them. The labelling follows Gaston *et al.* (2007) and the symbol '$\stackrel{\text{def}}{=}$' stays for definitions. For complete list of indices and their mutual relationships see SI.2

Definition	**Name, source and phenomenon**	
$J \stackrel{\text{def}}{=} \frac{S_{X\cap Y}}{S_X + S_Y - S_{X\cap Y}}$	Jaccard index; Jaccard (1912) (reversed Turnover, Co-occurrence)	Eq. T1
$\beta_{Sim} \stackrel{\text{def}}{=} \frac{\min(S_X, S_Y) - S_{X\cap Y}}{\min(S_X, S_Y)}$	Simpson beta; Simpson (1943); Lennon *et al.* (2001) (reversed Nestedness)	Eq. T2
$\beta'_{Sim} \stackrel{\text{def}}{=} 1 - \beta_{Sim} = \frac{S_{X\cap Y}}{\min(S_X, S_Y)}$	reversed Simpson beta (Simpson nestedness); Šizling *et al.* (2016) (Nestedness)	Eq. T3
$\beta_G \stackrel{\text{def}}{=} \frac{S_X + S_Y - 2S_{X\cap Y}}{S_X + S_Y - S_{X\cap Y}}$	Gaston beta, Koleff *et al.* (2003) (Turnover)	Eq. T4
$\beta_{Sør} \stackrel{\text{def}}{=} \frac{2S_{X\cap Y}}{S_X + S_Y}$	Sørensen index, Sørensen (1948) (reversed Turnover, Co-occurrence)	Eq. T5
$\beta_t \stackrel{\text{def}}{=} \frac{S_X + S_Y - 2S_{X\cap Y}}{S_X + S_Y} = 1 - \beta_{Sor}$	Wilson & Shmida (1984); labelled as in Gaston *et al.* (2007) Baselga (2010) calls this index Sørensen (Turnover)	Eq. T6
$\beta_{gl} \stackrel{\text{def}}{=} 2\frac{\lvert S_X - S_Y \rvert}{S_X + S_Y}$	Gaston & Lennon index of Species-Richness gradient; Lennon *et al.* (2001) (SI.3.T14) (Species-Richness Gradient)	Eq. T7
$\beta_{Wh} \stackrel{\text{def}}{=} 2\frac{S_X + S_Y - S_{X\cap Y}}{S_X + S_Y}$	Whittaker index of beta-diversity for two *adjacent* assemblages, Gaston *et al.* (2007) (Beta-diversity)	Eq. T8

Table 2: Table of possible inferences from variation of pairwise indices along temporal, geographic, or environmental gradients. Inference can be obtained from the comparison of the properties that vary (significant) with the properties which are constant (insignificant) along a given gradient. Some inference can be based on variation of a single index, regardless of other indices (first three rows in the table), but more specific inferences follow from a situation when one index significantly changes, while another index reveals only small variation (all remaining rows).

Variation along a gradient		Inference
Yes (Significant)	**No (Insignificant)**	
J	Whatever	change in turnover between regions/periods, change in co-occurrence, change in proportion of common species relative to alpha diversity;
β'_{Sim}	Whatever	change in nestedness comparedbetween regions/periods (i.e. nestedness for region 1 vs nestedness for region 2), change in proportion of common species relative to richness of species poorer sites (this change may or may not be induced only by change in the list of species of species-richer sites)
R	Whatever	change in species richness gradient (uniformity) between regions/periods; change in spatial variation of alpha diversity
β'_{Sim}	S_{rich}	Change in nestedess between regions/periods is driven by exchange of species at species poor sites
$\langle S \rangle$	S_{rich}	Difference of alpha diversity between regions/periods is driven by sites with fewer species
$\langle S \rangle$	S_{poor}	Difference of alpha diversity between regions/periods is driven by species-richer sites
R	$\langle S \rangle$	Regions/periods differ in spatial variation of alpha diversity without change of its average value
β'_{Sim}	J	Change in nestedness but not turnover/co-occurrence; Simultaneous change in lists of species that are unique to species-richer and species-poorer sites; variation in β'_{Sim}, no change in J, and Eq. 7 induce necessarily a change in R
J	β'_{Sim}, S_{poor}	Change in turnover/co-occurrence but not nestedness; change in list of species that are unique to species-richer sites; necessarily a change in R

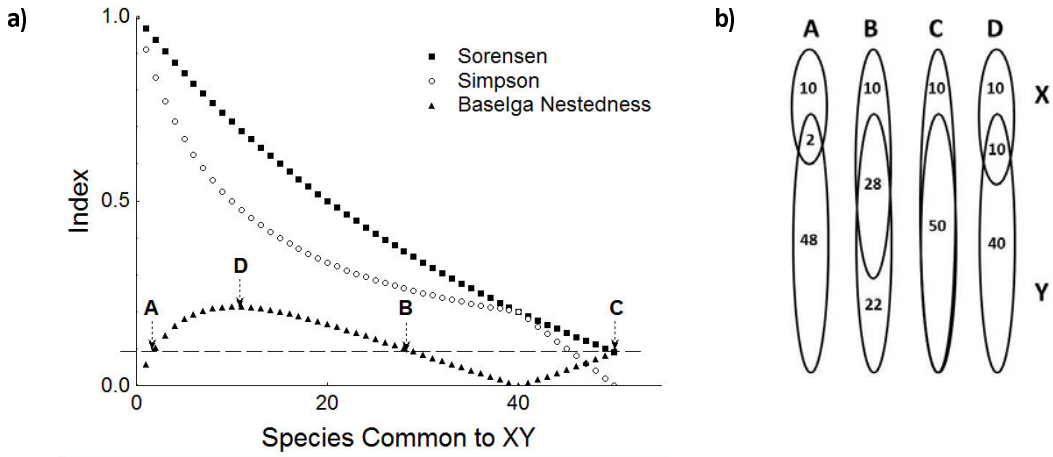

Fig. 1: (a) Simpson beta (β_{Sim}, circles, Table 1), reversed Sørensen index (β_t, squares, Table 1), and Nestedness by Baselga (here labelled as β_{Bas} but elsewhere as β_{nes}, triangles, Table 1) plotted against $S_{X\cap Y}$ for assemblages where $S_X = 50$ and $S_Y = 10 + S_{X\cap Y}$. β_{Bas} is zero, where the species lists have no species in common, $S_{X\cap Y} = 0$, and where each assemblage has 10 unique species ($S_{X\cap Y} = 40$). The arrows A-D point to the cases as shown in the subplot (b). **(b)** Four pairs of assemblages X,Y presented as Venn diagrams with numbers of species. The overlap between the sets shows the number of common species. The first three columns (A-C) show pairs of assemblages with equal $\beta_{Bas} = 0.1 \pm 0.01$. These cases include the absolutely nested arrangement (C). Unlike in C, the arrangement with maximum $\beta_{Bas} \cong 0.214$ across all possible arrangements (D) is not maximally nested according to the conceptual definition of nestedness. β_{Bas} behaviour is thus inconsistent along the gradient of increasing overlap in species ($S_{X\cap Y}$), all other parameters being equal. Consequently, β_{Bas} reaches the same values for very different situations, which is not desiderable for any consistent measure. See SI.1 for further details.

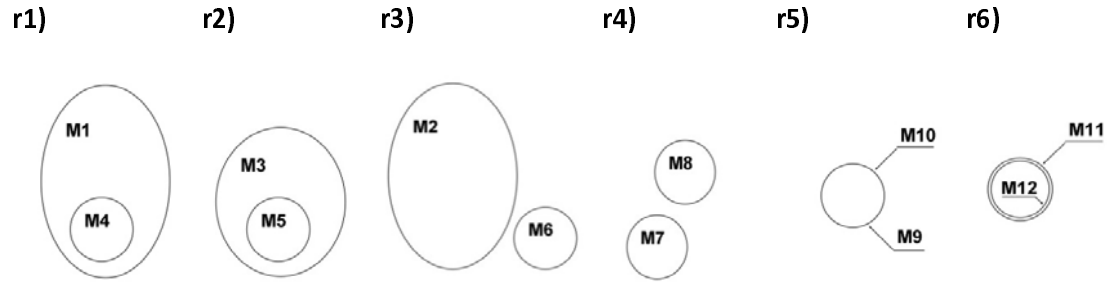

Fig. 2: Constraints by the five spatial phenomena on the indices. Various re-arrangements of two sets in the Venn diagrams define differences between the phenomena. The scheme equally applies to re-arrangements of two lists of species and two species spatial ranges, for the sets that would represent either lists of species or species spatial ranges, respectively. The sizes of the sets follow M1 = M2 > M3 > M4 = M5 = M6 = M7 = M8 = M9 = M10 =M11>M12. The sets M9 and M10 are identical. The constraints that define the five spatial phenomena are than as follows:

(Nestedness) $\mathrm{Min} = \mathrm{Nest}[\mathrm{r4}] = \mathrm{Nest}[\mathrm{r3}] < Nest[\mathrm{r1}] = \mathrm{Nest}[\mathrm{r2}] = \mathrm{Nest}[\mathrm{r6}] = \mathrm{Max} = \mathrm{Nest}[\mathrm{r5}]$;
(Co-occurrence) $\mathrm{Min} = \mathrm{Co}[\mathrm{r4}] = \mathrm{Co}[\mathrm{r3}] < Co[\mathrm{r1}] < Co[\mathrm{r2}] < Co[\mathrm{r6}] < Co[\mathrm{r5}] = \mathrm{Max}$;
(β-diversity) $\mathrm{Min} = \mathrm{BD}[\mathrm{r5}] < BD[\mathrm{r6}] < BD[\mathrm{r2}] < BD[\mathrm{r1}]$;
(Turnover) $\mathrm{Min} = \mathrm{Turn}[\mathrm{r5}] < Turn[\mathrm{r6}] < Turn[\mathrm{r2}] < Turn[\mathrm{r1}] < Turn[\mathrm{r4}] \leq \mathrm{Turn}[\mathrm{r3}]$; and
(sr-gradient) $\mathrm{Min} = \mathrm{SRG}[\mathrm{r5}] = \mathrm{SRG}[\mathrm{r4}] < SRG[\mathrm{r6}] < SRG[\mathrm{r2}] < SRG[\mathrm{r1}] = \mathrm{SRG}[\mathrm{r3}]$.

Where '*Min*' and '*Max*' label the extreme values of the focal indices (usually *Min*=0 and *Max*=1) and the letters in brackets refer to the re-arrangements. Every index that we test here must be defined in all cases, otherwise additional constraints have to be defined.

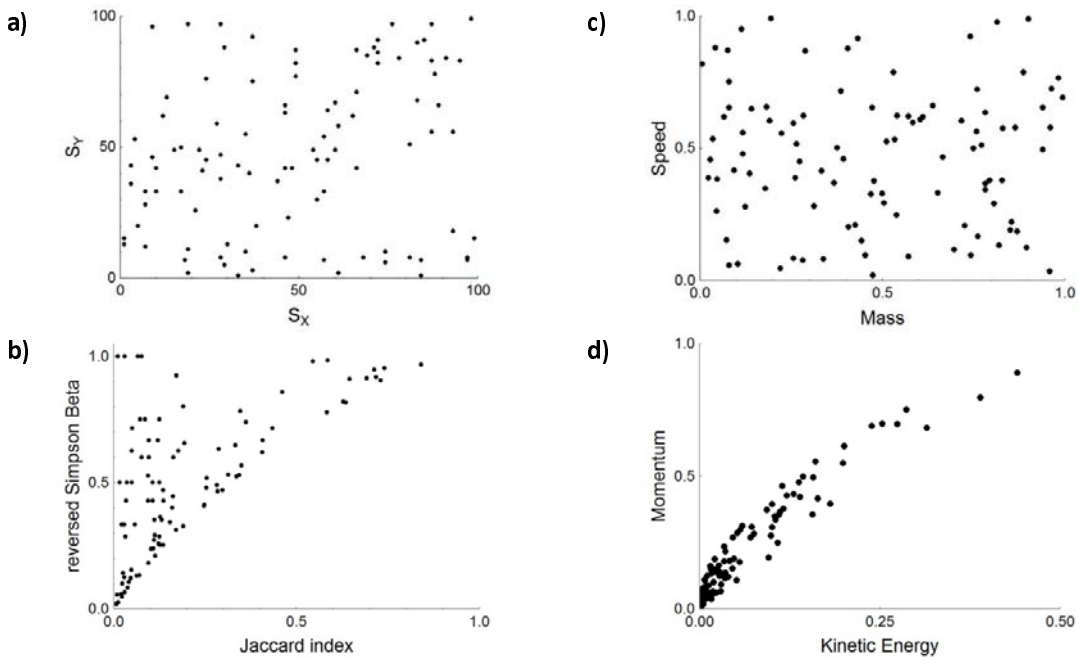

Fig. 3: Mutually statistically independent (s-independent) values for species assemblages in ecology (S_X and S_Y; **a**) and moving subjects in physics (mass and speed; **c**) do not necessarily result in statistically independent indices (J and β'_{Sim}; **b**) and variables (p and E_k; **d**). This is despite J, β'_{Sim}, p, and E_k carrying a specific information and therefore being independent (i-independent) regarding their information value. Here S_X, S_Y, ($\in \{1, \cdots, 100\}$) and $S_{X \cap Y}$ ($\leq \min\,(S_X, S_Y)$) are drawn at random from a uniform distribution (function 'trunc(rnd(99.9999)+1')).

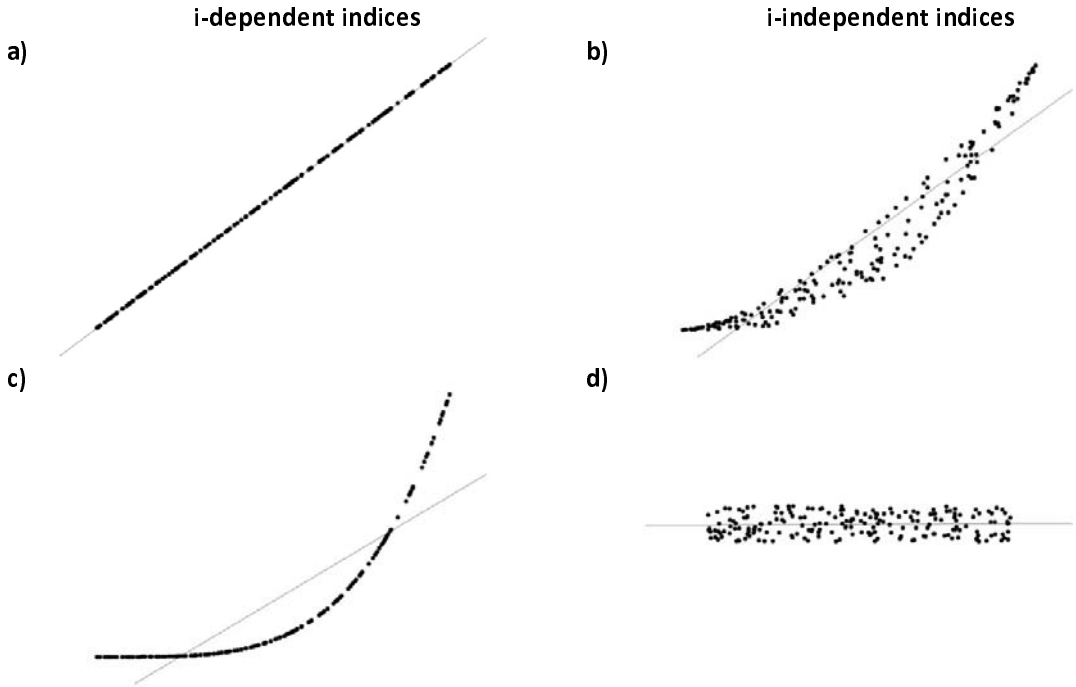

Fig. 4: An example of relationships between two i-dependent (a,c), i-independent (b,d), s-dependent (a-c), and s-independent (d) indices. Dots show 200 samples from the underlying relationships and lines show linear regressions. The underlying relationships between the i-dependent indices (a,c) are bijections, that is, one-to-one (strictly increasing) lines. The existence of these lines must be proven by means of mathematical analysis using the formulae that define the indices. But, there are apparently no one-to-one (strictly increasing nor decreasing) continuous lines beyond the samples of i-independent indices (b,d) (which does not require analytical proof). Only the indices in panel a) scale in a linear manner. The indices in panel c) are continuous (non-linear) transformations of each other. This transformation is called homeomorphism. Indices in panels b) and d) can also be viewed as transformations of each other, but this transformation is not a homeomorphism and thus each index may or may not measure different phenomena, depending on the constraints (Fig. 2). Degree of s-dependence measured by Pearson correlation coefficient decreases from a) to d) (1; 0.95; 0.86; 0; N=200). The i-dependences and i-independences are equal for a) and c), and b) and d), respectively.

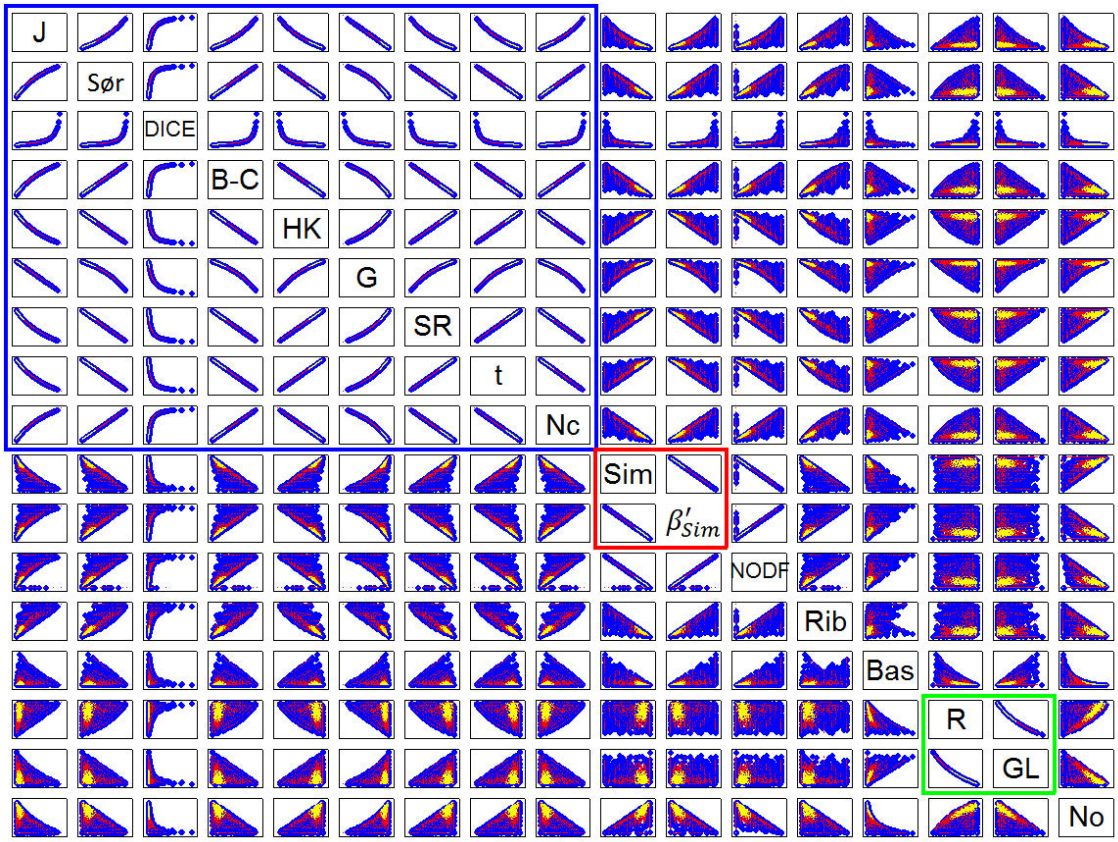

Fig. 5: Relationships between the indices for pairs of simulated random (blue dots, N=1352) and observed (red – plants, N=946; yellow – Ice Shield microbes, N=406) assemblages (see SI.7,SI.9 for data sources). The species richness values of assemblages in each pair are uncorrelated, i.e., numbers $S_{X\cap Y}$, $b = S_X - S_{X\cap Y}$ and $c = S_Y - S_{X\cap Y}$ vary between 0 and 1, they are drawn from a uniform distribution and are mutually s-independent. In N_0 and N_{NODF} (i.e., where the equality between S_X and S_Y affects the result) species richness is a random integer between 1 and 20 species. Where possible the notation is adapted from Gaston *et al.* (2007). The notation in the plot is simplified. From up to down: J – Table 1, β_{Sor} – Table 1, β_{DICE} - Raup & Crick (1979), β_{BC} – Bray & Curtis (1957) (computed for incidences), β_{HK} – Harte & Kinzig (1997), β_G – Table 1, β_{SR} – Schluter & Ricklefs (1993), β_t – Table 1, N_C - Wright & Reeves (1992) standardized as in Gotelli & McCabe (2002), β_{Sim} – Table 1, β'_{Sim} - Table 1, it equals *rN* (range nestedness, Šizling *et al.*, 2009) if applied to assemblages, β_{rib} – Ruggiero *et al.* (1998), β_{Bas}, called β_{nes} in Baselga (2010), R – Eq. 6; β_{gl} – Table 1, N_0 - Patterson & Atmar (1986), N_{NODF} - Almeida-Neto *et al.* (2008). Blue, red, yellow and green rectangles delimit the families of Jaccard-index, Simpson-beta, and species-richness gradient, respectively.

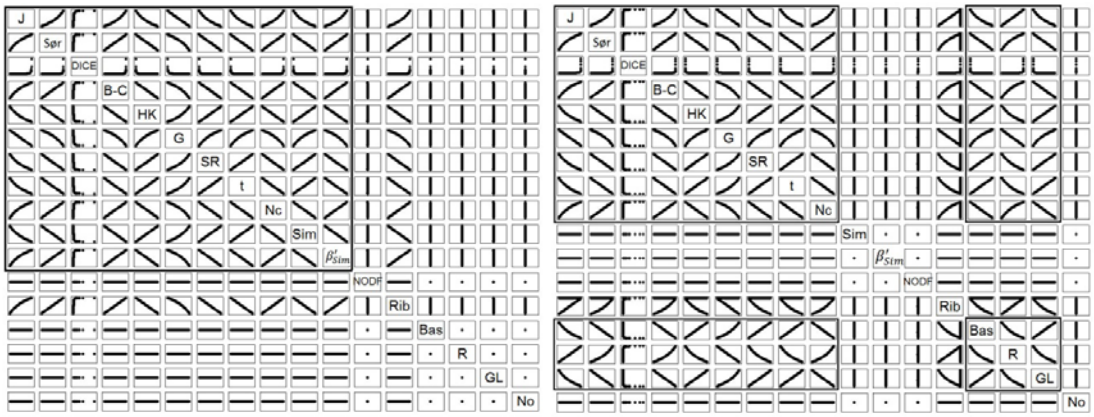

Fig. 6: Relationship between pairwise indices where there is no variation in species richness (a) and where assemblages are perfectly nested (b). As predicted, no variation in species richness merges families of J, β_{Sim} and N_0 together, and perfect nestedness merges families of J, β_{rb}, β_{Bas}, and β_{gl}. The evidence that β_{Bas} shows variability where nestedness is perfect disqualifies this measure from being a proxy for nestedness. Black rectangles delimit the merged families. For detailed legend see capture to Fig. 5.

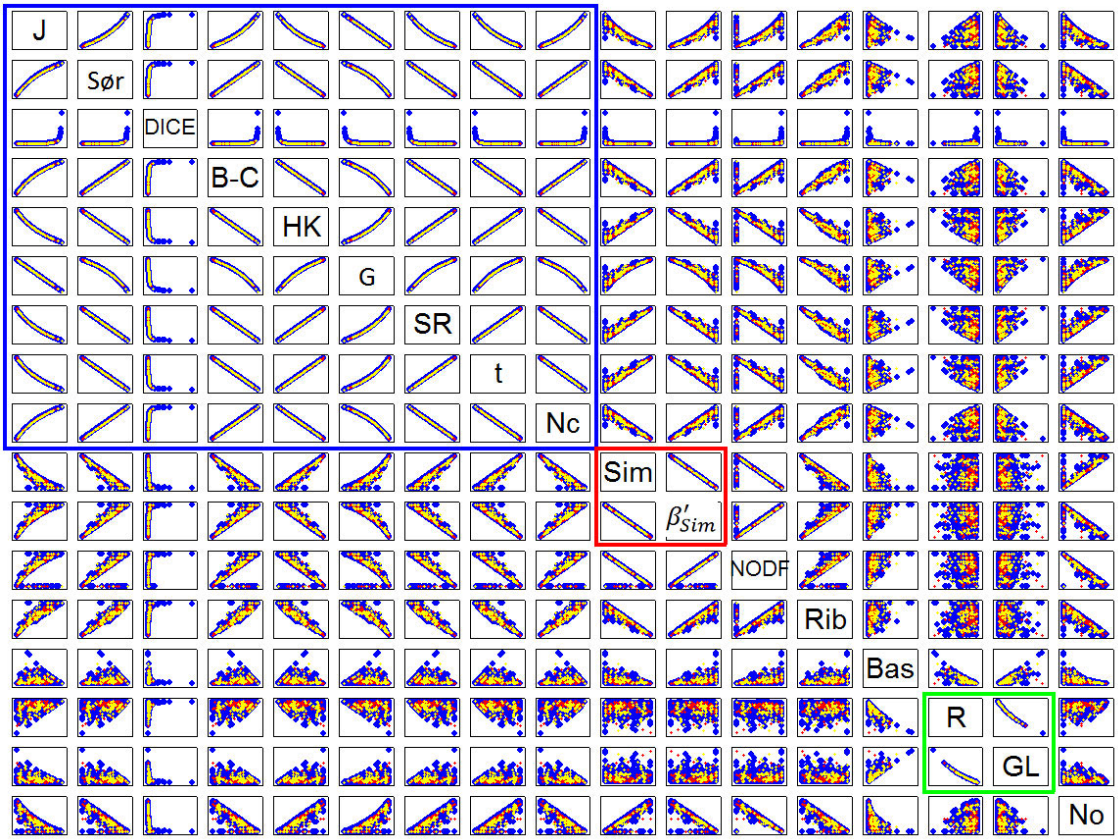

Fig. 7: Relationships between pairwise indices of assemblages which have low (20%) species richness variation (simulations) or which are spatially close to each other (observed data). Blue (N=1254) and yellow (N=98) dots show data generated by the simulations of random assemblages, and red dots show data for the plant and Ice-Shield microbe assemblages that are closer than 0.5 km from each other (N=98). The cluster of yellow dots is a random subsample of the blue dots, with N equal to the observation to allow comparison. In accord with the theory, when there is low variation in species richness or when the assemblages are close to each other, the Jaccard-index, Simpson-beta, Ruggiero-beta, and N_0 families collapse together into one big family of almost i-dependent (and definitely s-dependent) indices. For the meaning of abbreviations and colors see the legend to Fig. 5.

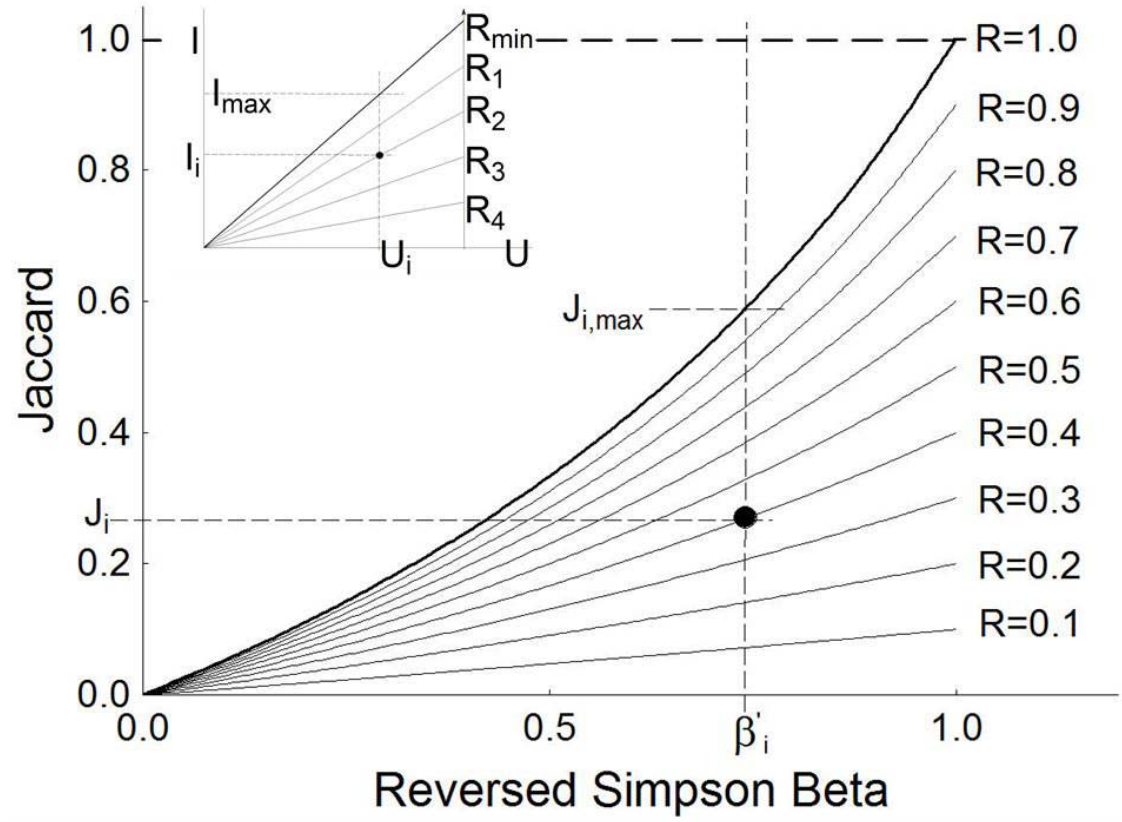

Fig. 8: The relationship between Jaccard (J) and reversed Simpson beta (β'_{Sim}) is determined by species richness uniformity R (Eq. 11), each line shows points with equal R (the dot has R=0.4). J is limited by 1 (dashed bold line) and each particular J_i is limited by $J_{i,max}$, which is a function of β'_{Sim} (bold line, Eq. 11). The value of J_i relative to the limit of one should be read as similarity (or reversed turnover) without a need for any partitioning of J or β'_{Sim} into components. We say that J is a similarity *per se* (or reversed turnover *per se*). The value J_i rescaled by $J_{i,max}$ shows R_i, and should be read as evenness *per se* (or reversed species richness gradient *per se*). The fact that *R* affects *J* is a matter of i-dependence between triplet J,β'_{Sim},*R*, and thus the interplay between *J* and *R* should not invalidate their unique meaning determined by the constraints (section 'Constraints needed to define the phenomena'). This is somehow similar to the Ohm's law in physics where the triplet of voltage (*U*), current (*I*) and resistance (*R*) are mutually dependent (*U=RI*; see inset). Each *I* is therefore affected by *R* (R_{1-4}, for the dot $R = R_2$) and has its upper limit given by technological limits to produce a component of low resistance (R_{min}, bold line). Most importantly, the understanding in physics is that I_i is the current even though it also scales with resistance. In the same way, J_i is reversed turnover per se even though it also scales with reversed richness gradient per se. For the same reason β'_{Sim} is a measure of nestedness per se, without a need for partitioning into components of turnover and/or nestedness.

Box 1: *How many indices do we need?*

For a given system, multitude of indices can be calculated. What is the minimum number of indices that characterize a given system fully? Here we show that three i-independent indices (including species richness) are sufficient for full characterization of the system, so that any other index can be reconstructed using this information. We adopt the term of independence from mathematics, which is independence of equations in terms of their solutions (hereafter i-independence). For this purpose, we need to see definitions of the indices as equations to solve. This allows for two statements: (i) all the focal indices listed in SI.2 are i-dependent on the pair of Jaccard index, *J* (Eq.T1 in Table 1) and Simpson nestedness, β'_{Sim} (Eq.T3); and (ii) all information concerning the contrast between two assemblages is captured by *J*, β'_{Sim}, and an index that is i-dependent on species richness. Here we show why these statements hold.

All the focal indices of diversity (SI.2) can be defined as a ratio of two linear functions

$$I \stackrel{\text{def}}{=} \frac{k_1 S_{X\cap Y}+k_2 S_X+k_3 S_Y}{l_1 S_{X\cap Y}+l_2 S_X+l_3 S_Y}, \quad (k_{1-3},\ l_{1-3} \in \boldsymbol{R}),\ \ |l_2|+|l_3|>0\,, S_X \geq S_Y > 0. \qquad \text{(Eq. B1)}$$

For *J* and β'_{Sim}, $\{k_{1-3}, l_{1-3}\}$={1,0,0,-1,1,1} and {1,0,0,0,0,1}, respectively. Following the logic: $I = \frac{a}{b} \ \rightarrow bI - a = 0$, Eq. B1 can be converted into linear equation

$$S_X(Il_2 - k_2) + S_Y(Il_3 - k_3) + S_{X\cap Y}(Il_1 - k_1) = 0, \qquad \text{(Eq. B2)}$$

where S_X, S_Y, $S_{X\cap Y}$ are the unknowns and the *I* is a particular value of an index. Eq. B2 turns into

$$S_X J + S_Y J - S_{X\cap Y}(J+1) = 0 \text{ and } S_Y \beta'_{Sim} - S_{X\cap Y} = 0 \qquad \text{(Eq. B3)}$$

for *J* and β'_{Sim}, respectively. The two equations for two indices (Eq. B3), and the three unknown variables (S_X, S_Y, $S_{X\cap Y}$), do not provide a unique solution, and have zero at the right side. If the third equation had zero on the right side, the system would either provide multiple solutions or the only solution would be zero ($S_X, S_Y, S_{X\cap Y} = 0, 0, 0$). We therefore need an independent equation with nonzero right side to get unique information on S_X, S_Y, $S_{X\cap Y}$. This equation is

$$S_X + S_Y = 2\langle S\rangle, \qquad \text{(Eq. B4)}$$

where $\langle S\rangle \neq 0$ is the expected species richness of one assemblage, that is, the mean richness (for the proof that Eq. B4 is independent of equations B3, see SI.3.T1). The three equations (Eqs. B3,B4) determine $S_X, S_Y, S_{X\cap Y}$ uniquely, and thus no other index (even if its definition does not follow B1) can further specify the solution. Moreover, if we restrict our statements on the existing indices which can be expressed using Eq. B1, we can compute the value of any other index from the values of *J* and β'_{Sim} as

$$I = \frac{J(\beta'_{Sim}(k_1+k_2)-k_2+k_3)+\beta'_{Sim}k_2}{J(\beta'_{Sim}(l_1+l_2)-l_2+l_3)+\beta'_{Sim}l_2}, \qquad \text{(Eq. B5)}$$

where k_i, l_i define the new index *I* (for proof see **SI3.T16**). For *I*=*R*, we substitute $\{k_{1-3}, l_{1-3}\}$={0,0,1,0,1,0} and Eq. B5 turns into Eq. 6.

Box 2: *How to unify indices from across the literature*

A large number of different indices is spread over the literature (e.g., Legendre & Legendre, 2012). However, if one wishes to do a meta-analysis and compare indices from different published sources, one needs to make the indices comparable, and to convert them to only one or two reference indices. Here we show how this can be done, based on the idea that an index is defined by an equation. Firstly, we need a publication using at least two i-independent indices, I_1, I_2, that are expressed as Eq. B1. Then we write a system of three independent equations: two equations B2, each for one of the indices, and one scaling equation Eq. B3. If $\langle S \rangle$ is missing from the publication, we can put $\langle S \rangle = 1$ without loss of generality. The reason is that the indices to be converted (Eq. B1) are i-independent of species richness and therefore the exact value of $\langle S \rangle$ does not matter in the case. The third equation then is

$$S_X + S_Y = 2. \tag{B7}$$

The solution of the three equations (See SI.3.T18 for the guide how to solve them) is S_{Xcomp}, S_{Ycomp} and $S_{X \cap Ycomp}$. This solution is different from the solution based on the original data behind the published source, but we can get the original average values S_{Xorig}, S_{Yorig}, $S_{X \cap Yorig}$ by simple rescaling of the computed values ($S_{Xorig} = \langle S \rangle S_{Xcomp}$ and so on), in case we know $\langle S \rangle$. From S_{Xcomp}, S_{Ycomp}, $S_{X \cap Ycomp}$ we can compute any index that is i-independent of species richness, even an index that cannot be expressed as Eq. B1 (e.g., $I = S_X S_{X \cap Y} / S_Y^2$).

A special case is β_{Bas}, which cannot be directly expressed as Eq. B1. The β_{Bas} is, however, defined as difference between two indices from Jaccard and Simpson families, and therefore cannot carry more information than J and β'_{Sim} (or another two mutually i-independent indices that are i-independent of species richness, see Box 1). If one of the published indices is β_{Bas}, we need to convert the second published index into β_t or β_{Sim} (see SI.2 for equations to convert). If we have β_{Sim}, we compute β_t as $\beta_{Bas} - \beta_{Sim}$ – if we have β_t, we compute β_{Sim} as $\beta_{Bas} - \beta_t$. Then we continue as instructed earlier in this box with one equation for β_{Sim}, second equation for β_t and third equation B7. If the published source uses β_{Bas} and an index convertible to R (Eq. 6), we simply use the formula

$$\beta_{Bas} = \frac{(R^{-1} - 1) S_{X \cap Y}}{S_X + S_Y} \tag{B8}$$

(see SI.3.T19 for derivation). This formula follows Eq. B1 and thus can be converted into linear equation $\beta_{Bas} S_X + \beta_{Bas} S_Y + (1 - R^{-1}) S_{X \cap Y} = 0$, which is i-independent of the equation for R ($R S_X - S_Y = 0$; $S_Y \leq S_X$). We then again continue with these two equations and Eq. B7 following the instructions above.