Biodiversity Patterns along Ecological Gradients: Unifying β-Diversity Indices

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Abstract
Ecologists have developed an abundance of conceptions and mathematical expressions to define β-diversity, the link between local (α) and regional-scale (γ) richness, in order to characterize patterns of biodiversity along ecological (i.e., spatial and environmental) gradients. These patterns are often realized by regression of β-diversity indices against one or more ecological gradients. This practice, however, is subject to two shortcomings that can undermine the validity of the biodiversity patterns. First, many β-diversity indices are constrained to range between fixed lower and upper limits. As such, regression analysis of β-diversity indices against ecological gradients can result in regression curves that extend beyond these mathematical constraints, thus creating an interpretational dilemma. Second, despite being a function of the same measured α- and γ-diversity, the resultant biodiversity pattern depends on the choice of β-diversity index. We propose a simple logistic transformation that rids beta-diversity indices of their mathematical constraints, thus eliminating the possibility of an uninterpretable regression curve. Moreover, this transformation results in identical biodiversity patterns for three commonly used classical beta-diversity indices. As a result, this transformation eliminates the difficulties of both shortcomings, while allowing the researcher to use whichever beta-diversity index deemed most appropriate. We believe this method can help unify the study of biodiversity patterns along ecological gradients.

Introduction
Ecologists have long expressed interest in spatial and environmental effects on biodiversity, specifically the effects with respect to β-diversity, which quantifies the similarity of species assemblage among sites and represents the link between local (α) diversity and regional (γ) diversity [1]. Consensus on a standard definition of β-diversity, however, has been elusive and has been the subject of considerable debate – both in terms of its fundamental essence [1–5] and its mathematical relationship with α- and γ-diversity [2,4,6–8]. Much mathematical discussion revolves on whether β-diversity is defined better by a multiplicative (i.e., αβM = γ) [9] or an additive (i.e., α + βA = γ) [10,11] partition.

Over time, many different expressions for “β-diversity” have been proposed, which, in addition to considerable ambiguous terminology, has led to confusion within the ecological community [2,4,12]. Although each expression addresses the compositional similarity among sites, each is also a different measure of compositional similarity and thus, describes a somewhat different concept. The choice of beta-diversity index is, therefore, dependent on the researcher’s ecological application [4]. One set of beta-diversity indices, the “classical metrics” [1], defines α-diversity in terms of the mean diversity in local sites and γ-diversity as the composite of these local sites.

One popular approach to quantify spatial or environmental patterns of biodiversity is regression analysis of a classical β-diversity index against one or more spatial or environmental gradients [13–19]. This approach, however, is subject to two shortcomings that can undermine the validity of the resultant diversity patterns. First, classical β-diversity indices are mathematically constrained, i.e., each index features a lower limit when all local sites are compositionally the same and an upper limit when all local sites are unique. Regression of such β-diversity indices can result in a predicted estimation that crosses these limits, thus violating their mathematical constraints. Such instances cast doubt on the validity of the regression diagnostics, e.g., correlation, residuals, t-tests etc. Second, the regression analysis is dependent on the choice of β-diversity index, thus a biodiversity pattern resulting from one β-diversity index may be radically different from another β-diversity index.

We introduce a simple transformation that rids commonly used classical β-diversity indices of their lower and upper constraints, thereby eliminating the risk of regression analysis producing non-interpretable regression curves. Moreover, regression of these transformed indices against spatial or environmental gradients yields identical relationships for these commonly used classical β-diversity indices. As a result, this transformation eliminates the difficulties of both shortcomings, while allowing the researcher to use whichever β-diversity index deemed most appropriate.
Table 1. Mathematical definitions and expressions of beta-diversity indices.

| β-index | Function | Low | High |
|---------|----------|-----|------|
| δ_Md   | γ/x     | 1   | N    |
| δ_Md-1 | (γ−x)/x | 0   | N−1  |
| δ_Pt   | (γ−x)/γ | 0   | 1−(1/N) |

Low and High represent the lower and upper limits of beta-diversity indices as a function of the number of local sites (N).
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Methods: Mathematical Properties of Logistic-Transformed β-Diversity Indices

Classical β-diversity indices are derived from the measured local diversity (x) – usually expressed as the arithmetic mean of species richness in N local sites – and regional diversity (γ), the measured species richness of all N local sites combined. β-diversity is often expressed by one of three β-diversity indices, which are described here using the terminology in Tuomisto [4]. True β-diversity, δ_Md, expressed as γ/x, quantifies the number of compositional units in the collection. δ_Md is equivalent to δ_Mt, the basic multiplicative diversity partition. δ_Md-1, expressed as γ/x−1, provides the number of complete turnovers among the compositional units in the collection. Proportional species turnover, δ_Pt, expressed as (γ−x)/γ, described the proportion of species found regionally that are not found locally.

All three β-diversity indices, δ_Md, δ_Md-1, and δ_Pt, assume a minimum value when all local sites are compositionally identical and a maximum when all local sites are compositionally unique. The lower limit for δ_Md and δ_Pt is zero and for δ_Md unity. The respective upper limits are a function of N (Table 1).

A logistic transformation (γ = ln[x/(1−x)]) is a standard method by which to treat data that are constrained by upper and lower limits [20]. An analogous transformation applied to these β-diversity indices takes the generalized form, β̂ = ln [(δ_Md−δ_Mmin)/(δ_Mmax−δ_Mmin)], where δ_Mmax and δ_Mmin are the respective upper and lower limit of a β-diversity index, β. Index β̂ can be recovered from β̂ by β = exp(β̂)/(1 + exp(β̂))(δ_Mmax−δ_Mmin)+

Table 2. Values of γ- and x-diversity along a hypothetical ecological gradient for three scenarios.

| Gradient | Scenario | γ  | a(A) | a(B) | a(C) |
|----------|----------|----|------|------|------|
| 1        | A        | 10 | 9.5  | 2    | 9.5  |
| 2        | B        | 20 | 18.6 | 6    | 10   |
| 3        | C        | 40 | 34   | 6    | 38   |
| 4        | A        | 30 | 18   | 10.5 | 9    |
| 5        | B        | 50 | 37.5 | 17.5 | 31.2 |
| 6        | C        | 80 | 24   | 12   | 46.5 |
| 7        | A        | 70 | 21   | 8.4  | 14   |
| 8        | B        | 100| 12   | 12   | 40   |
| 9        | C        | 80 | 9.6  | 12   | 24   |
| 10       | A        | 90 | 13.5 | 9.9  | 35.8 |

Figure 1. Scatterplots of beta-diversity indices against hypothetical ecological gradient for Scenario A. (a) δ_Md (left axis) and δ_Md-1 (right axis); linear regression trends, |δ_Md| γ = 0.87x−1.17, for |δ_Md|, y = 0.87x−2.17 (r = 0.88 for both). (b) δ_Pt linear regression trend, y = 0.11x−0.10 (r = 0.95). (c) δ_Md, δ_Md-1 (circles) and δ_Pt (squares); linear regression trends, for |δ_Md|, β̂ = 0.78x−6.10, for δ_Pt, y = 0.78x−3.80 (r = 0.91 for all). Dashed trends in (a) and (b) depict linear trends of γ̂ (and β̂_Md-1) and δ̂_Pt retransformed to δ_Md (and δ_Md-1) and δ_Pt, respectively. See Table 1 for description of beta-diversity indices and Table 2 for data for Scenario A.
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β̂_Mn: This retransformation allows the depiction of beta-diversity in its more familiar constrained units, as a logistic variable may be difficult to visualize. The beta-diversity relationship with a gradient can be plotted simply as the retransformed β̂ as a function of the gradient. Any value of β̂ will — upon retransformation into β — adhere to the mathematical constraint, β̂_Mn ≤ β ≤ β̂_Mn. Given, for example, a set of N = 10 local sites with x = 50 and γ = 100,
are (squares); linear regression trends, for \( \beta_\text{Md}^* \), \( \beta_\text{Pt}^* \), \( \beta_{\text{Md}1} \), and \( \beta_{\text{Pt}1} \) are 2, 1, and 0.5, respectively. Corresponding values of \( \beta_{\text{Md}1}^* \) and \( \beta_{\text{Pt}1}^* \) are \(-2.08\), \(-2.08\), and \(0.22\), respectively. Note that because \( \beta_{\text{Md}} = \beta_{\text{Md}1} = 1 \), \( \beta_{\text{Md1}} = \beta_{\text{Md1}}^* \), and that \( \beta_{\text{Pt}} = \beta_{\text{Pt1}} + \ln(N) = \beta_{\text{Pt1}} + \ln(N) \).

**Results: Illustrative Example**

Table 2 provides a set of illustrative data of \( \alpha \)- and \( \gamma \)-diversity along a hypothetical environmental or spatial gradient to compare the performance of these commonly used classical \( \beta \)-diversity indices with their logistic-transformed equivalents. Ten points along the gradient were assigned values of \( \gamma \) and different values of \( \alpha \) for three scenarios. In all scenarios, \( N = 10 \), thus the upper limits for \( \beta_{\text{Md}} \), \( \beta_{\text{Md1}} \), and \( \beta_{\text{Pt}} \) are 10, 9, and 0.9, respectively.

In Scenario A, \( \beta_{\text{Md}} \), \( \beta_{\text{Md1}} \), and \( \beta_{\text{Pt}} \) all exhibit a statistically significant positive relationship along the gradient. The linear regression curves of \( \beta_{\text{Md}} \) and \( \beta_{\text{Md1}} \) cross below the lower limits, 1 and 0 respectively, at gradient values \( < \sim 3 \) (Figure 1a). The linear regression curve of \( \beta_{\text{Pt}} \) derived from the same set of \( \alpha \) and \( \gamma \), crosses the upper limit at gradient values \( > \sim 9 \) (Figure 1b). In other words, Scenario A provides an example of two different \( \beta \)-diversity indices violating their mathematical constraints at opposite ends of the gradient. The logistic-transformed equivalents, \( \beta_{\text{Md}}^* \), \( \beta_{\text{Md1}}^* \), and \( \beta_{\text{Pt}}^* \), when regressed along the gradient yield statistically significant linear relationships with identical values for all regression parameters except for the intercept (Figure 1c). The intercept of \( \beta_{\text{Pt}}^* \) is 2.30 greater than that of \( \beta_{\text{Md}}^* \) and \( \beta_{\text{Md1}}^* \), which is equivalent to \( \exp(N) \), i.e., \( \exp(10) \). Moreover, the resultant regression curves when retransformed into their original \( \beta \)-diversity indices adhere to their respective upper and lower constraints (Figure 1a, b).

The linear regression curves of \( \beta_{\text{Md}} \), \( \beta_{\text{Md1}} \), and \( \beta_{\text{Pt}} \) in Scenarios B and C all lie within the upper and lower limits. However, the relationship between \( \beta_{\text{Pt}} \) and the gradient in Scenario B is statistically significant at 95% confidence (\( p = 0.026 \)), whereas those between \( \beta_{\text{Md}} \) and \( \beta_{\text{Md1}} \) are non-significant (\( p = 0.097 \)) (Figure 2a). This result is opposite in Scenario C: the relationship between \( \beta_{\text{Pt}} \) and the gradient is statistically non-significant (\( p = 0.121 \)), whereas those between \( \beta_{\text{Md}} \) and \( \beta_{\text{Md1}} \) are significant (\( p = 0.036 \)) (Figure 2b). In addition, the magnitude of the residuals in Scenarios B and C differ between \( \beta_{\text{Md}} \) (or \( \beta_{\text{Md1}} \)) and \( \beta_{\text{Pt}} \). By contrast, linear regression of \( \beta_{\text{Md}}^* \), \( \beta_{\text{Md1}}^* \), and \( \beta_{\text{Pt}}^* \) against the gradient results in identical models for both Scenario B and C with the exception of their respective intercepts. The relationship is significant for both Scenario B (\( p = 0.023 \)) and Scenario C (\( p = 0.039 \)) and both relationships are independent of the choice of \( \beta \)-diversity index. In addition, this choice has no effect on the resultant residual patterns (Figure 2c, d).

**Discussion**

Space structure is an often neglected consideration in statistical analysis. All conventional multivariate statistical analysis assume that the data occupy Euclidean space [21], yet this is rarely the case. A constrained space structure can usually be readily
transformed into Euclidean space; log-transformation of positive-only data is a well-known example. Likewise, logistic transformation can be used to place data constrained by upper and lower limits into an unbounded line in Real space. Logistic transformation is commonly used for data restricted to values between one and unity (as in odds ratios) [20,22], but can also be performed on constrained classical β-diversity indices. As our illustrative example shows, regression analysis of “raw” classical β-diversity indices can result in regression curves that violate their imposed mathematical constraints, thereby undermining the validity of the regression model and its interpretation. By contrast, regression of logistic-transformed β-diversity indices excludes the possibility of violating these mathematical constraints, thereby eliminating any “impossible” results that would undermine the regression model.

Logistic transformation also eliminates the effects of the choice of these classical β-diversity indices. Although regression of βMd and βMd-1 results in identical diversity patterns (the intercept using βMd-1 is one less than that using βMd), neither is equivalent to βPn, which results in a different diversity pattern. This dilemma is especially worrisome; it seems intuitive that a single measured set of $\alpha$- and $\gamma$-diversity should lead to a unique diversity pattern even if β-diversity is expressed by different indices. Our illustrative example shows that a diversity pattern along an ecological gradient can be statistically significant using one index and non-significant using another. Even if the interpretational contrast is not so dramatic, the difference among β-diversity indices can still affect the residuals, which can influence outlier detection, particularly when data points lie close to the limits. By contrast, logistic transformation results in a unique diversity pattern for all three logistic-transformed indices. The difference between βMd and $\beta_M^{Md-1}$ and $\beta_P^{Md-1}$ is simply a function of the number of local sites. As a result, all regression parameters (except the intercept) are identical for all β-diversity indices.

Although the illustrative examples shown reflect simple linear regression relationships, the two advantages of the logistic transformation are maintained regardless of the actual relationship, i.e. even if the relationship between logistic-transformed beta-diversity and ecological gradient is markedly non-linear. As a result, the researcher is free to choose any appropriate regression model, including many non-linear models, to describe the beta-diversity pattern. For instance, a polynomial or piecewise (i.e., segmented) regression model could be used to characterize a unimodal relationship. Positive-only regression models, such as logarithmic and exponential models, are excluded, because logistic beta-diversity indices can assume negative values. The lack of equivalency among the “raw” classical beta-diversity indices can lead to inconsistency in describing even the qualitative nature of biodiversity patterns. For example, whereas the relationship of $\beta_P$ with the gradient in Figure 2b is linear, the relationship with $\beta_M^{Md}$ and $M^{Md-1}$ is arguably non-linear (Figure 2a). As a result, using $\beta_M^{Md}$ or $\beta_M^{Md-1}$ could lead to the conclusion that beta diversity increases only along the upper part of the gradient, whereas using $\beta_P$ suggests that beta-diversity increases along the entire gradient.

The lack of equivalency notwithstanding, attempts to circumvent the constraints on classical β-diversity indices by other methods are fraught with difficulty. For instance, the arc-sine transformation, despite its long tradition of use to mitigate constrained data such as percentage data, has been the subject of criticism and is rapidly running out of favour [22–24]. Moreover, the results of regression on arcsine transformed indices remains dependent on the choice of index. Regression of logistic-transformed indices typically presumes that the data contain no regions in which all the local sites are either unique or identical; logistic transformation is impossible for a data point located exactly on an upper or lower limit. However, methods are available to perform regression analysis based on a logistic-transformed response variable that includes otherwise non-transformable data [25,26].

Although we have demonstrated the use of logistic transformation on the regression of classical β-diversity indices, the transformation can also be used to circumvent violation of the constraints of pairwise “multivariate measures” [1], such as the Jaccard and Sørensen indices, which are constrained to values between 0 and 1. The Jaccard and Sørensen indices are equivalent to $\beta_P$ and $\beta_M^{Md-1}$, respectively, for a pair of sites. As such, the logistic transformation can also result in a unique diversity pattern for the Jaccard and Sørensen indices. Logistic-transformation of β-diversity indices is not limited to simple presence-absence estimates with $\alpha$-diversity calculated as the arithmetic mean. A similar approach can be followed by expressing $\alpha$-diversity as a geometric mean, as the maximum richness in a set of local sites [27,29], or by expressing diversity in terms of “effective numbers of species”, which incorporates species abundance [29–31]. “Effective numbers of species” can be calculated from, for instance, Shannon or Simpson indices. Moreover, the method can also be applied to phylogenetic and functional richness [32]. We suggest the logical transformation of β-diversity indices as a means of improving and simplifying the interpretation of diversity patterns along ecological gradients.

Author Contributions
Conceived and designed the experiments: RS MP. Performed the experiments: RS. Analyzed the data: RS. Contributed reagents/materials/analysis tools: RS MP. Wrote the paper: RS MP.

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