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Multiple site dissimilarity quantifies compositional heterogeneity among several sites, while average pairwise dissimilarity may be misleading

Andrés Baselga

A. Baselga (andres.baselga@usc.es), Depto de Zoología, Facultad de Biología, Univ. de Santiago de Compostela, c/Lope Gómez de Marzoa s/n, ES-15782 Santiago de Compostela, Spain.

Several measures of multiple site dissimilarity have been proposed to quantify the overall heterogeneity in assemblage composition among any number of sites. It is also a common practice to quantify such overall heterogeneity by averaging pairwise dissimilarities between all pairs of sites in the pool. However, pairwise dissimilarities do not account for patterns of co-occurrence among more than two sites. In consequence, the average of pairwise dissimilarities may not accurately reflect the overall compositional heterogeneity within a pool of more than two sites. Here I use several idealized examples to illustrate why pairwise dissimilarity measures fail to properly quantify overall heterogeneity. Thereafter, the effect of this potential problem in empirical patterns is exemplified with data of world amphibians. In conclusion, when the attribute of interest is the overall heterogeneity in a pool of sites (i.e. beta diversity) or its turnover or nestedness components, only multiple site dissimilarity measures are recommended.

Several debates have recently contributed to clarify concepts underlying beta diversity and, more generally, the patterns of biotic dissimilarity among species assemblages. Major debates have addressed the need for clear terms and definitions (Jurasinski et al. 2009, Tuomisto 2010, Anderson et al. 2011), the independence of beta diversity measures from alpha and gamma diversities (Jost 2007, Ricotta 2008, Baselga 2010a, Veech and Crist 2010, Chao et al. 2012), and the contribution of spatial turnover (species replacement) and nestedness to beta diversity (Baselga 2010b, Podani and Schmera 2011, Almeida-Neto et al. 2012, Baselga 2012). During these debates, a number of insights have been gained about the link between classical pairwise measures of dissimilarity (quantifying how different two assemblages are) and beta diversity *sensu stricto* (i.e. gamma/alpha, Tuomisto 2010). Several pairwise dissimilarity indices are just monotonic transformations of beta diversity for the special case of two sites (Jost 2007). The underlying reason is that gamma diversity differs from alpha diversity if, and only if, local assemblages differ in species composition. Therefore, for a pool of two assemblages, biotic heterogeneity can be quantified using a pairwise dissimilarity measure.

When the question of interest is how heterogeneous the species composition is among several assemblages (i.e. more than 2 sites, times or, in general, units), we are addressing an attribute of the whole pool of units. In other words, beta diversity is an attribute of the pool (region, time period...), not of any of the units within the pool. This

attribute can be quantified by measuring the multiple site dissimilarity among units. However, another widely used practice has been averaging pairwise dissimilarity between all pairs of units in the pool. The rationale behind is the intuitive idea that the integration of the pairwise dissimilarities between all pairs of units has to be a measure of total heterogeneity or, in a slightly different approach, that multivariate dispersion in multidimensional space is a measure of total variation in species composition (Anderson et al. 2006). This approach is widespread and the averaged pairwise dissimilarities have been repeatedly used as a measure of regional heterogeneity in empirical analyses (Gaston et al. 2007, McKnight et al. 2007, Melo et al. 2009, Leprieur et al. 2011) and even proposed in new methodological approaches to quantify the overall heterogeneity across multiple sites (see Podani and Schmera 2011, Jurasinski et al. 2012 for different approaches) and presented as an alternative measure of beta diversity in conceptual reviews (Anderson et al. 2011).

However, as Diserud and Ødegaard (2007) have explicitly shown, pairwise indices ignore the information about patterns of co-occurrence in more than two sites and therefore are not appropriate for measuring biotic heterogeneity across more than two sites. Given that, despite Diserud and Ødegaard's (2007) key contribution, the use of averaged pairwise dissimilarities is still a widespread procedure, the aim of this note is to stress why multiple site (or, more generally, multiple unit) measures are necessary when the attribute of interest is the overall heterogeneity corresponding to a

pool of $n > 2$ sites (units). To do this, I provide 1) several simple idealized cases showing that averaged pairwise measures are blind to the patterns of co-occurrence among more than two sites, despite these patterns would be responsible of total heterogeneity and, 2) a case study with world amphibian species to assess the potential bias when using averaged pairwise indices in empirical studies. All calculations were performed in R (R Development Core Team) using the packages betapart (Baselga and Orme 2012) and vegan (Oksanen et al. 2011). The dissimilarity measures used in all cases were the pairwise and multiple site versions of the Sørensen dissimilarity index (β_{sor} and β_{SOR} , respectively), and their turnover (Simpson index of dissimilarity, β_{sim} and β_{SIM} , respectively) and nestedness (nestedness-resultant index of dissimilarity, β_{sne} and β_{SNE} , respectively) components (Baselga 2010b, 2012).

Does averaged pairwise dissimilarity reflect total heterogeneity in the pool?

Different amounts of strict sense beta diversity (i.e. gamma/alpha) in a pool of $n > 2$ units can yield the same value for the average of pairwise dissimilarities or the average of distances to centroid in a multidimensional space (Fig. 1). This can occur independently of whether variation in species composition is caused by spatial turnover (species replacement from site to site) or nestedness (species loss from site to site, so poorer assemblages are subsets of richer assemblages). For example, in the two situations described in Fig. 1a, b, all sites are equally rich and dissimilarity between sites is completely due to spatial turnover. In both cases, two species are shared between any pair of sites and

one species is unique to each site of the pair. For this reason, the average of pairwise dissimilarities takes the same value in both situations (mean $\beta_{sor} = \beta_{sim} = 0.33$), as it does the mean distance to the centroid in a multidimensional space ($z = 0.20$, as computed with the betadisper function in vegan). However, while no species is unique to a single site in Fig. 1a, one species is unique to each site in Fig. 1b. This is captured by the strict sense measure of beta diversity ($\beta_W = \gamma/\alpha$), or by the multiple site dissimilarity measures that allow separating the turnover and nestedness components ($\beta_{SIM} = \beta_{SOR}$, in this case, because beta diversity is completely due to spatial turnover). Therefore, the multiple site measures consider that biotic heterogeneity is greater in Fig. 1b than in Fig. 1a. In the absence of spatial turnover, when nestedness is the pattern behind biotic heterogeneity (Fig. 1c, d), the same disconnection between averaged pairwise values and multiple site measures can be observed. In Fig. 1c only one species is unique to a single site, with the other species being shared by two or more sites, whereas in Fig. 1d three species are unique to a single site, with the remaining species being shared between the four sites. Whittaker's beta (β_W) or the multiple site dissimilarity measures ($\beta_{SNE} = \beta_{SOR}$, in this case) suggest that biotic heterogeneity is greater in Fig. 1d than in Fig. 1c but, in turn, the averaged pairwise dissimilarities or the mean distance to the centroid are larger in Fig. 1c than in Fig. 1d.

It could be argued that such a discrepant behavior of multiple site and averaged pairwise dissimilarities would stem from different definitions of biotic heterogeneity and that no objective benchmark exists to decide, for example, whether the biotas described in Fig. 1b are more heterogeneous than those in Fig. 1a. However, I would like to stress that the strict sense definition of beta diversity (β_W)

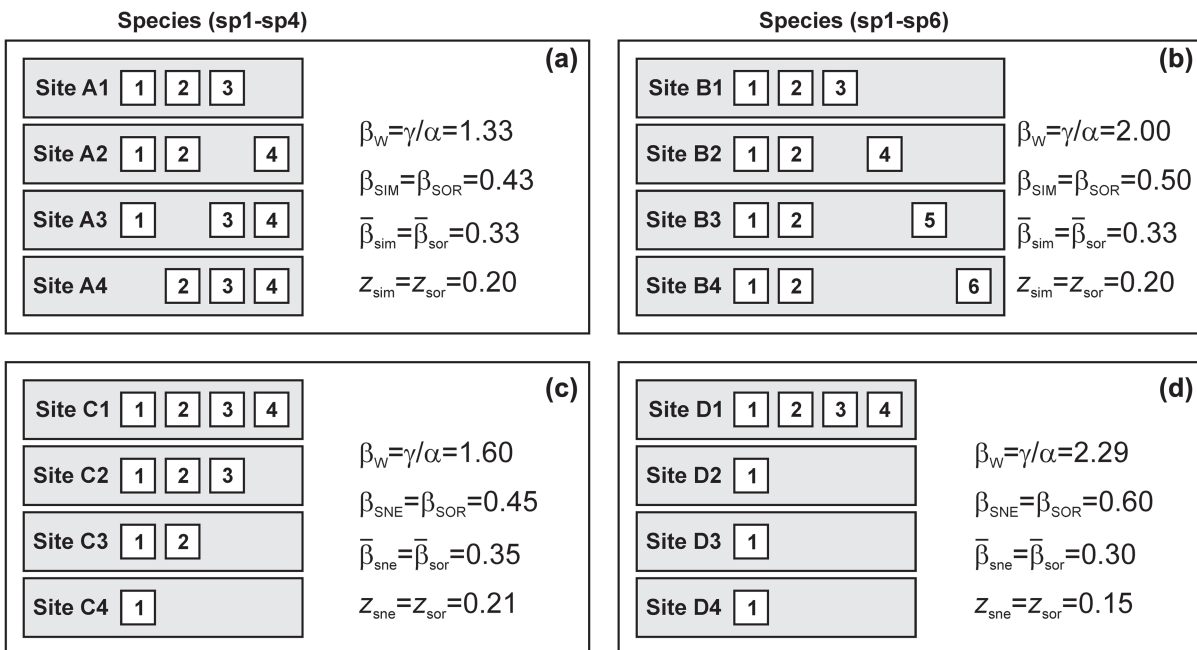


Figure 1. Hypothetical examples showing the discrepancy between multiple site and averaged pairwise measures in contexts where biotic heterogeneity is completely derived from spatial turnover (a, b) or nestedness (c, d). Strict sense beta diversity (β_W), multiple site dissimilarity (β_{SOR} , β_{SIM} , β_{SNE}), averaged pairwise dissimilarity (β_{sor} , β_{sim} , β_{sne}) and distance to centroid of the multivariate space defined by pairwise dissimilarities (z) are provided.

is the ratio between gamma and alpha diversity (Whittaker 1960, Tuomisto 2010) and, therefore, β_W quantifies the effective number of different communities in the regional pool (Jost 2007). In fact, for beta diversity values being comparable between systems with different number of sites, β_W has to be transformed to make it independent of the number of sites. The transformed measure is in fact a multiple site generalization of the Sørensen index (Chao et al. 2012), i.e. the proportion of unique species per site. In the examples, because the number of sites in Fig. 1a, b is the same, and because the effective number of different communities in Fig. 1b is higher than in Fig. 1a, the conclusion that biotic heterogeneity is higher in Fig. 1b than in Fig. 1a is unavoidable, in my opinion. In general terms, this provides a benchmark: biotic heterogeneity is univocally linked to the strict sense definition of beta diversity.

The lack of concordance between the amount of variation in composition among more than two sites and the mean value of pairwise dissimilarities arises from the fundamental fact that pairwise dissimilarities are, by definition, unable to account for patterns of co-occurrence involving more than two sites, as already pointed by Diserud and Ødegaard (2007). In other words, when the composition of several sites is compared by pairs using pairwise dissimilarity measures, the information about how many species are shared or not by several sites or how many unique species there are with respect to several sites is completely ignored. However, the total amount of compositional heterogeneity among $n > 2$ sites (i.e. beta diversity) depends on the patterns of co-occurrence involving all the n sites. Thus, multiple site dissimilarity measures are mandatory if the specific question to be addressed is the measurement of total variation in species composition in more than two sites or, in other words, how heterogeneous species composition is in a pool of n units. Needless to say, pairwise dissimilarity measures are a perfectly valid method for many other questions, i.e. distance decay of similarity, cluster analysis and ordinations, among others.

Among multiple site measures of compositional variation, it should be noted that the classical multiplicative beta diversity (Whittaker 1960) or its n -independent transformation (i.e. the multiple-site generalization of the Sørensen index; Chao et al. 2012) do a perfect job for measuring overall biotic heterogeneity among more than two sites. However, the aforementioned measures are unable to discern whether biotic heterogeneity is derived from species replacement form site to site, from nested patterns or from both. Therefore, in order to simultaneously allow 1) accounting for patterns of co-occurrence among more than two sites and 2) partitioning overall biotic heterogeneity into turnover and nestedness components, two families of multiple site measures derived from Sørensen ($\beta_{SOR} = \beta_{SIM} + \beta_{SNE}$) and Jaccard indices ($\beta_{JAC} = \beta_{JTU} + \beta_{JNE}$) have been developed (Baselga 2010b, 2012).

Does it matter in the real world?

The next question to be answered is to which extent measuring total biotic heterogeneity with averaged pairwise dissimilarities does introduce a bias in empirical patterns.

Geographical patterns in beta diversity of world amphibians represent an excellent case study due to the strong variation in beta diversity across the world, the high number of cases that can be compared and the clear latitudinal patterns in both the turnover and nestedness components of beta diversity (Baselga et al. 2012). Therefore, I measured the concordance (Spearman rank correlation, ρ) between multiple site dissimilarity components derived from turnover or nestedness (β_{SIM} or β_{SNE} , respectively) and the equivalent averaged pairwise dissimilarities (mean β_{sim} or mean β_{sne} , respectively), calculated in all cases for the pool of $1^\circ \times 1^\circ$ cells contained within regional squares of 250 000 km² (Sastre et al. 2009). Spearman rank correlation was selected to account for non-linear relationships. Given that multiple site measures had to be standardized to a determined number units ($n = 15$, for more details see Baselga et al. 2012), the same resampling procedure was implemented for averaged pairwise measures to guarantee full comparability (i.e. 15 $1^\circ \times 1^\circ$ cells were randomly sampled within each large regional square and the average of pairwise dissimilarities was computed 10 times). Thereafter, I assessed the existence of breakpoints in latitudinal gradients of beta diversity (see Baselga et al. 2012 for details). In short, I performed a set of piecewise regressions between components of beta diversity and absolute latitude and selected the breakpoint that yielded the lowest residual standard error (Crawley 2007).

When the global results for multiple site and pairwise dissimilarities are compared (Fig. 2a, b), it turns out that multiple site (β_{SIM}) and averaged pairwise measures (mean β_{sim}) are highly correlated for turnover ($\rho = 0.99$, $p < 0.001$), but only moderately correlated for nestedness-resultant dissimilarity ($\rho = 0.67$, $p < 0.001$). It should be noted that the concordance or lack of concordance is case-specific, and things could be even worse, especially when beta diversity is high, as suggested by the greater scatter in the upper right quadrant of Fig. 2a, b. This is because both multiple site and averaged pairwise measures have to be unavoidably small for lower levels of biotic heterogeneity but, for higher levels of biotic heterogeneity, the concordance is lost. As an example, if we were interested in amphibian beta diversity patterns in the Andean region ($n = 18$ regional squares), the correlation between multiple site and averaged pairwise measures (Fig. 2c, d) would be much lower in the case of turnover ($\rho = 0.74$, $p < 0.001$) and even more in the case of nestedness-resultant dissimilarity ($\rho = 0.59$, $p = 0.011$). Thus, in this specific case, the use of averaged pairwise measures would probably yield completely biased patterns that would not reflect the real relationships between beta diversity and the underlying topographic, climatic and historical factors. Remarkably, such cases where beta diversity is high are precisely the most interesting ones for studying its relationship with potential determinants.

Moreover, despite the high correlation observed for the global dataset, the marked latitudinal breakpoint observed with the multiple site measures (Fig. 3a, c) is not clearly recovered using averaged pairwise measures (Fig. 2c, d). For turnover, averaged pairwise measures still detect the existence of a breakpoint ($F_{2, 301} = 39.5$, $p < 0.001$) at the same latitude (37°), although the proportion of variation explained is significantly reduced compared to the model for

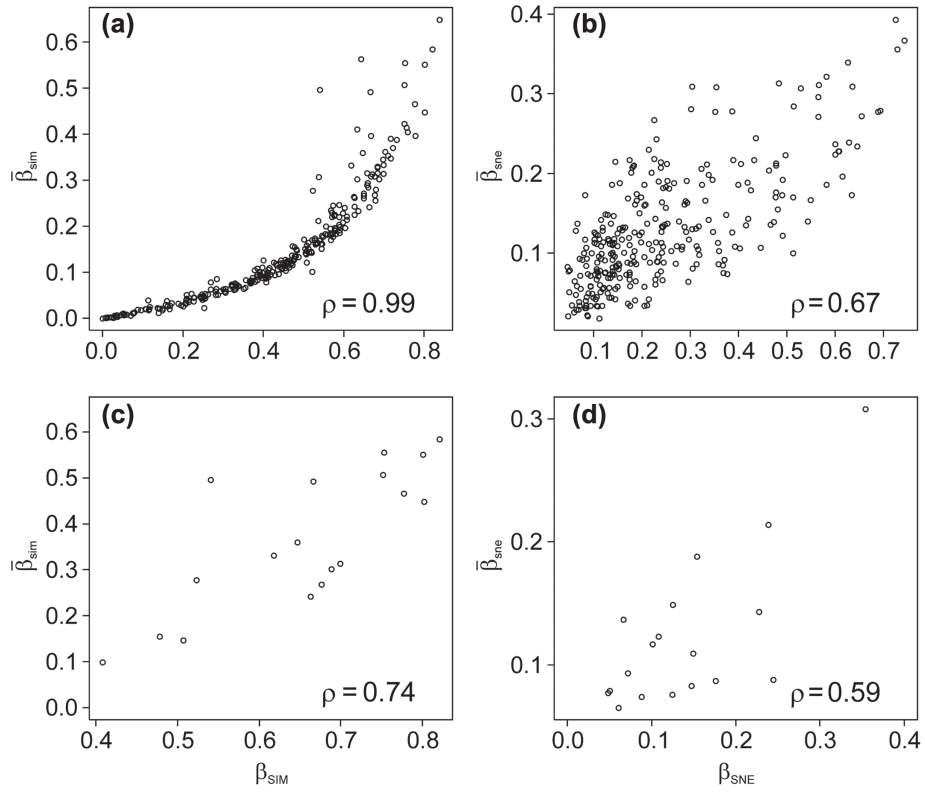


Figure 2. Relationship between multiple site and averaged pairwise dissimilarities in amphibian assemblages across the world (a, b) and the Andean region (c, d). Both multiple site and pairwise dissimilarity were partitioned into its turnover, (β_{SIM} and mean β_{sim} , respectively; (a, c)) and nestedness components (β_{SNE} and mean β_{sne} ; (b, d)).

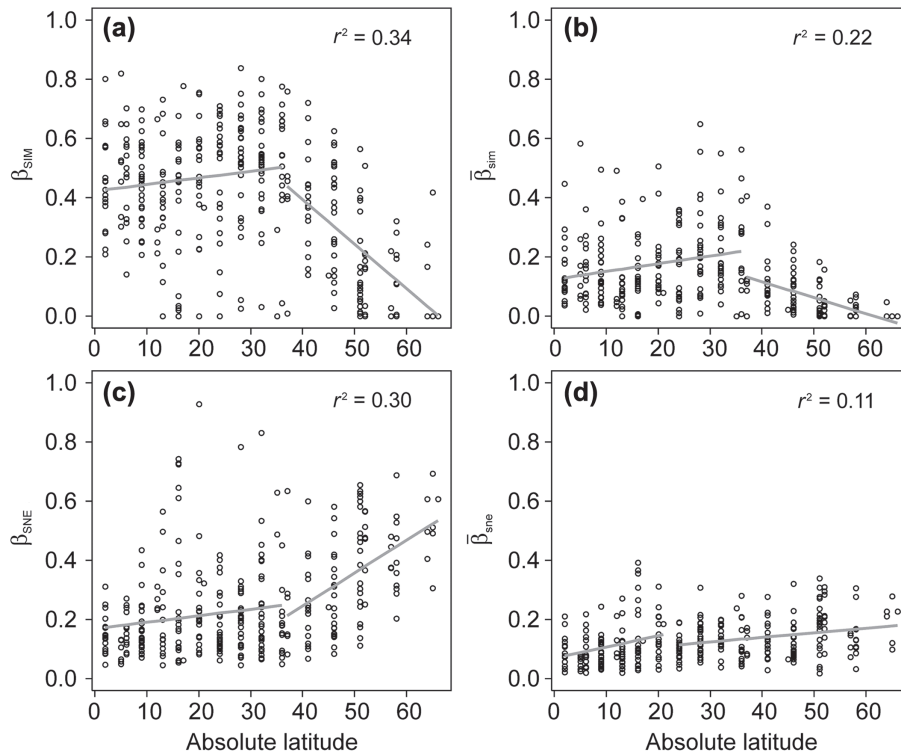


Figure 3. Latitudinal patterns in turnover (a, b) and nestedness-resultant dissimilarity (c, d) as measured by multiple site dissimilarity (a, c) and averaged pairwise dissimilarity measures (b, d).

multiple site β_{SIM} (i.e. r^2 drops from 0.34 to 0.22). In the case of nestedness-resultant dissimilarity, the pattern is almost lost when using averaged pairwise dissimilarities, as the breakpoint ($F_{2, 301} = 17.6$, $p < 0.001$) is recovered at a different latitude and the proportion of variation explained is much lower (r^2 drops from 0.30 to 0.11).

To conclude, the simple idealized cases presented above (Fig. 1) exemplify that pairwise dissimilarity measures are inappropriate to quantify the overall compositional heterogeneity among a set on $n > 2$ units. This is because overall heterogeneity depends on patterns of co-occurrence involving all the n units within the pool for which heterogeneity is measured, while pairwise measures are blind to patterns of co-occurrence involving more than two units, by definition. In empirical patterns, especially when the range of heterogeneity is wide (i.e. the data include very homogeneous and very heterogeneous regions) the pattern yielded by averaged pairwise measures would probably present a certain degree of correlation with the actual multiple site dissimilarity pattern. However, this correlation could be low, especially in systems of high heterogeneity, which are indeed the most meaningful ones when assessing the potential drivers of change in biotic composition. Thus, when the attribute of interest is the overall assemblage heterogeneity in a pool of units (i.e. beta diversity) or its turnover or nestedness components, only multiple site dissimilarity measures are recommended.

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References

- Almeida-Neto, M. et al. 2012. Rethinking the relationship between nestedness and beta diversity: a comment on Baselga (2010). – *Global Ecol. Biogeogr.* 21: 772–777.
- Anderson, M. J. et al. 2006. Multivariate dispersion as a measure of beta diversity. – *Ecol. Lett.* 9: 683–693.
- Anderson, M. J. et al. 2011. Navigating the multiple meanings of beta diversity: a roadmap for the practicing ecologist. – *Ecol. Lett.* 14: 19–28.
- Baselga, A. 2010a. Multiplicative partition of true diversity yields independent alpha and beta components, additive partition does not. – *Ecology* 91: 1974–1981.
- Baselga, A. 2010b. Partitioning the turnover and nestedness components of beta diversity. – *Global Ecol. Biogeogr.* 19: 134–143.
- Baselga, A. 2012. The relationship between species replacement, dissimilarity derived from nestedness, and nestedness. – *Global Ecol. Biogeogr.* 21: 1223–1232.
- Baselga, A. and Orme, C. D. L. 2012. betapart: an R package for the study of beta diversity. – *Methods Ecol. Evol.* 3: 808–812.
- Baselga, A. et al. 2012. Historical legacies in world amphibian diversity revealed by the turnover and nestedness components of beta diversity. – *PLoS One* 7: e32341.
- Chao, A. et al. 2012. Proposing a resolution to debates on diversity partitioning. – *Ecology* 39: 2037–2051.
- Crawley, M. J. 2007. *The R book*. – Wiley.
- Diserud, O. H. and Ødegaard, F. 2007. A multiple-site similarity measure. – *Biol. Lett.* 3: 20–22.
- Gaston, K. J. et al. 2007. Spatial turnover in the global avifauna. – *Proc. R. Soc. B* 274: 1567–1574.
- Jost, L. 2007. Partitioning diversity into independent alpha and beta components. – *Ecology* 88: 2427–2439.
- Jurasinski, G. et al. 2009. Inventory, differentiation, and proportional diversity: a consistent terminology for quantifying species diversity. – *Oecologia* 159: 15–26.
- Jurasinski, G. et al. 2012. Detecting spatial patterns in species composition with multiple plot similarity coefficients and singularity measures. – *Ecography* 35: 73–88.
- Leprieux, F. et al. 2011. Partitioning global patterns of freshwater fish beta diversity reveals contrasting signatures of past climate changes. – *Ecol. Lett.* 14: 325–334.
- McKnight, M. W. et al. 2007. Putting beta-diversity on the map: broad-scale congruence and coincidence in the extremes. – *PLoS Biol.* 5: 2424–2432.
- Melo, A. S. et al. 2009. Environmental drivers of beta-diversity patterns in New-World birds and mammals. – *Ecography* 32: 226–236.
- Oksanen, J. et al. 2011. *vegan: community ecology package*. – R package ver. 2.0-2, <<http://cran.r-project.org/>>.
- Podani, J. and Schmera, D. 2011. A new conceptual and methodological framework for exploring and explaining pattern in presence–absence data. – *Oikos* 120: 1625–1638.
- Ricotta, C. 2008. Computing additive beta-diversity from presence and absence scores: a critique and alternative parameters. – *Theor. Popul. Biol.* 73: 244–249.
- Sastre, P. et al. 2009. A Geoplatform for the accessibility to environmental cartography. – *J. Biogeogr.* 36: 568.
- Tuomisto, H. 2010. A diversity of beta diversities: straightening up a concept gone awry. Part 1. Defining beta diversity as a function of alpha and gamma diversity. – *Ecography* 33: 2–22.
- Veech, J. A. and Crist, T. O. 2010. Diversity partitioning without statistical independence of alpha and beta. – *Ecology* 91: 1964–1969.
- Whittaker, R. H. 1960. Vegetation of the Siskiyou Mountains, Oregon and California. – *Ecol. Monogr.* 30: 280–338.