VARIATION PARTITIONING OF SPECIES DATA MATRICES: ESTIMATION AND COMPARISON OF FRACTIONS

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Abstract. Establishing relationships between species distributions and environmental characteristics is a major goal in the search for forces driving species distributions. Canonical ordinations such as redundancy analysis and canonical correspondence analysis are invaluable tools for modeling communities through environmental predictors. They provide the means for conducting direct explanatory analysis in which the association among species can be studied according to their common and unique relationships with the environmental variables and other sets of predictors of interest, such as spatial variables. Variation partitioning can then be used to test and determine the likelihood of these sets of predictors in explaining patterns in community structure. Although variation partitioning in canonical analysis is routinely used in ecological analysis, no effort has been reported in the literature to consider appropriate estimators so that comparisons between fractions or, eventually, between different canonical models are meaningful. In this paper, we show that variation partitioning as currently applied in canonical analysis is biased. We present appropriate unbiased estimators. In addition, we outline a statistical test to compare fractions in canonical analysis. The question addressed by the test is whether two fractions of variation are significantly different from each other. Such assessment provides an important step toward attaining an understanding of the factors patterning community structure. The test is shown to have correct Type I error rates and good power for both redundancy analysis and canonical correspondence analysis.

Key words: adjusted coefficient of determination; bootstrap; canonical analysis; canonical correspondence analysis (CCA); ecological community; redundancy analysis (RDA); variation partitioning.

INTRODUCTION

The search for causes dictating patterns in species distributions in natural and disturbed landscapes is of primary importance in ecological science, and establishing relationships between species distributions and environmental characteristics is a widely used approach (e.g., Legendre and Fortin 1989, Jackson and Harvey 1993, Diniz-Filho and Bini 1996, Rodríguez and Lewis 1997, Jenkins and Buikema 1998, Boyce and McDonald 1999, Peres-Neto and Jackson 2001). Habitat models relating habitat characteristics and community structure (species occurrence or abundance) are expected to answer at least two questions. (1) How well is the distribution of a set of species explained by the given set of predictive variables? (2) Which variables are irrelevant or redundant in the sense of failing to strengthen the explanation of patterns after certain other variables have been taken into account? The first question relates to the predictive power of the model that can be used in conservation management, for questions such as esti-

mating habitat suitability, forecasting the effects of habitat change due to human interference, establishing potential locations for species reintroduction, or predicting how community structure may be affected by the invasion of exotic species. The second question is important for heuristic issues such as determining the likelihood of competing hypotheses to explain particular patterns in community structure (Peres-Neto et al. 2001).

Canonical analyses such as redundancy analysis (RDA; Rao 1964), canonical correspondence analysis (CCA; ter Braak 1986), and distance-based redundancy analysis (db-RDA; Legendre and Anderson 1999) are invaluable tools for modeling communities through environmental predictors. They provide the means for conducting direct explanatory analyses in which the association among species can be studied with respect to their common and unique relationships with environmental variables or any other set of predictors of interest. As a demonstration of its success, well over 1500 studies applying CCA or RDA in modeling species–environment relationships have been published (see also Birks et al. [1996] for reviews on ecological studies using these methods). RDA and CCA can be best understood as methods for extending multiple regression that has a single response y and multiple predictors $\mathbf{X}$ (e.g., several environmental predictors), to
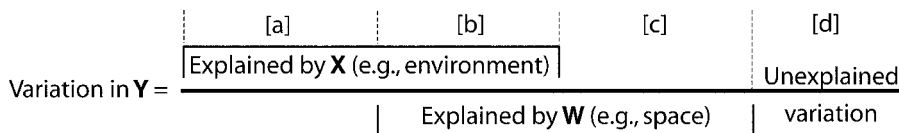
FIG. 1. Variation partitioning scheme of a response variable **Y** between two sets of predictors **X** (e.g., environmental factors) and **W** (e.g., spatial predictors). The total variation in **Y** is partitioned into four fractions as follows: (1) fraction [a + b + c] based on both sets of predictor matrices [**X,W**] ([a + b + c] = $R^2_{\mathbf{Y}|[\mathbf{X,W}]}$); (2) fraction [a + b] based on matrix **X** ([a + b] = $R^2_{\mathbf{Y}|\mathbf{X}}$); (3) fraction [b + c] based on matrix **W** ([b + c] = $R^2_{\mathbf{Y}|\mathbf{W}}$); (4) the unique fraction of variation explained by **X**, [a] = [a + b + c] − [b + c]; (5) the unique fraction of variation explained by **W**, [c] = [a + b + c] − [a + b]; (6) the common fraction of variation shared by **X** and **W**, [b] = [a + b + c] − [a] − [c]; and (7) the residual fraction of variation not explained by **X** and **W**, [d] = 1 − [a + b + c].

multiple regression involving multiple response variables **Y** (e.g., several species) and a common matrix of predictors **X**. It follows that the percentage of variation of the response matrix explained by the predictor matrix (hereafter referred to as the redundancy statistic, or simply $R^2_{\mathbf{Y}|\mathbf{X}}$ following Miller and Farr 1971) is the canonical equivalent of the regression coefficient of determination, R^2.

In multiple regression analysis, we can apply variation partitioning (also known as commonality analysis; Kerlinger and Pedhazur 1973) to identify common and unique contributions to model prediction and hence better address the question of the relative influences of the groups of independent variables considered in the model (Mood 1969). When partitioning variation is used in regression analysis, independent variables are grouped into sets representing broad factors. In that context, variation partitioning is more suitable than analyzing the individual contributions of regressors via their partial correlation coefficients. In this approach, the total percentage of variation explained by the model (R^2) is partitioned into unique and common contributions of the sets of predictors (Fig. 1). For example, variation partitioning for RDA or CCA using two sets of predictors (**X** and **W**) is straightforward as it is based on three canonical analysis (Fig. 1). The first one uses both sets of predictors [**X,W**], the second only **X**, and the last one only **W**. All remaining fractions of the partitioning can be obtained by simple subtractions (Fig. 1). Note that the shared variation ([b], Fig. 1) may be negative due to suppressor variables (i.e., a regressor having low, close to zero, correlation with the response variable and a correlation with another regressor, which in turn is correlated with the response variables; see Azen and Budescu [2003] for more details) or due to two strongly correlated predictors with strong effects on *y* of opposite signs (one positive and the other negative; Legendre and Legendre 1998: Section 10.3.5). Variation partitioning based on two sets of predictor matrices was introduced to canonical analysis by Borcard et al. (1992) and Borcard and Legendre (1994), later was extended to three or more sets of predictor matrices (Anderson and Gribble 1998, Cushman and McGarigal 2002, Økland 2003), and is now routinely used in direct gradient analysis.

Although canonical analysis and variation partitioning may provide a robust approach for understanding the relative influence of different ecological factors driving community assembly, judging the importance of a factor solely on the basis of its proportional unique contribution is not as straightforward as currently performed. The statistical bias related to estimating a population ρ^2 based on a sample R^2 is a well-recognized problem (Zar 1999), as sample estimates tend, on average, to be larger than ρ^2. The bias is influenced by both the number of independent variables in the model and sample size (Kromrey and Hines 1995). Terms such as adjustment and "shrinkage" refer to the fact that a sample-estimated R^2 needs to be reduced in order to provide a more accurate estimate of ρ^2. By taking into account the appropriate degrees of freedom, the adjustment provides a way of comparing models with different numbers of predictors (e.g., model selection) and sample sizes. Given that R^2 and $R^2_{\mathbf{Y}|\mathbf{X}}$ are intrinsically related, the bias observed in multiple regression also exists in canonical analysis. Although variation partitioning in canonical analysis is routinely used in ecological analysis, no effort has been reported in the literature to consider appropriate estimators so that comparisons between fractions or eventually between different canonical models are meaningful. Specifically, our objective is twofold: (1) to provide adjustments for the bias in sample $R^2_{\mathbf{Y}|\mathbf{X}}$, and (2) to outline a statistical test to contrast partial effects in canonical analysis (i.e., compare fractions of variation).

REDUNDANCY STATISTIC IN CANONICAL ANALYSIS

Here we present the formulation of the $R^2_{\mathbf{Y}|\mathbf{X}}$ statistic used in canonical analysis applied to species data matrices. In the case of RDA, $R^2_{\mathbf{Y}|\mathbf{X}}$ is calculated as follows:

$$R^2_{\mathbf{Y}|\mathbf{X}} = \frac{\text{trace}(\hat{\mathbf{Y}}'\hat{\mathbf{Y}})}{\text{trace}(\mathbf{Y}'_{\text{cent}}\mathbf{Y}_{\text{cent}})}$$

$$= 1 - \frac{\text{trace}[(\mathbf{Y}_{\text{cent}} - \hat{\mathbf{Y}})'(\mathbf{Y}_{\text{cent}} - \hat{\mathbf{Y}})]}{\text{trace}(\mathbf{Y}'_{\text{cent}}\mathbf{Y}_{\text{cent}})} \quad (1)$$

where $\hat{\mathbf{Y}} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}_{\text{cent}}$ represents the matrix of predicted values. Note that this is identical to calculating predicted values for individual multiple regressions of each column of **Y** on **X**; $\mathbf{Y}_{\text{cent}} = (\mathbf{I} - \mathbf{P})\mathbf{Y}$ is matrix **Y**

centered by column means (i.e., column means = 0). $\mathbf{I}$ is an $(n \times n)$ identity matrix and $\mathbf{P}$ is a $(n \times n)$ matrix with all elements = $1/n$; n refers to the number of sampling units. Matrix $\mathbf{X}$ can be either centered or standardized (column means = 0 and column variances = 1).

The definition of $R^2_{\mathbf{Y}|\mathbf{X}}$ presented here is the one used in ecological applications; it is called the RDA trace statistic in the Canoco program, Version 4.5 (ter Braak and Smilauer 2002) and the proportion of explained variation in Legendre and Legendre (1998). This definition is different from the one in redundancy analysis as used in behavioral research (Dawson-Saunders 1982, Lambert et al. 1988) where the response variables are standardized rather than centered prior to analysis. In that case, the $R^2_{\mathbf{Y}|\mathbf{X}}$ is simply the mean of the R^2 statistics computed for each individual multiple regression of each column of $\mathbf{Y}$ on matrix $\mathbf{X}$ (Miller 1975). In ecological analysis the species are centered and not standardized, so $R^2_{\mathbf{Y}|\mathbf{X}}$ is a weighted mean of the R^2 of individual models with weights proportional to the species variances divided by the total variance. The same definition based on a weighted mean applies to CCA, and for the sake of brevity we present the $R^2_{\mathbf{Y}|\mathbf{X}}$ used in CCA in Appendix A.

AN ADJUSTED REDUNDANCY STATISTIC FOR CANONICAL ANALYSIS—THE CONTINUOUS CASE

Our first task was to determine whether adjustments for the multiple coefficient of determination (R^2_{adj}) developed for a single response variable could also be applied to the canonical $R^2_{\mathbf{Y}|\mathbf{X}}$. Dawson-Saunders (1982) has shown that Ezekiel's adjustment (1930), commonly used in the case of multiple regressions (Legendre and Legendre 1998, Zar 1999), is appropriate for the case where response variables are standardized prior to analysis. Ezekiel's formulation applied to canonical analysis based on centered values is as follows:

$$R^2_{(\mathbf{Y}|\mathbf{X})\mathrm{adj}} = 1 - \frac{n-1}{n-p-1}(1 - R^2_{\mathbf{Y}|\mathbf{X}})$$

$$= 1 - \frac{\mathrm{trace}[(\mathbf{Y}_{\mathrm{cent}} - \hat{\mathbf{Y}})(\mathbf{Y}_{\mathrm{cent}} - \hat{\mathbf{Y}})]/(n-p-1)}{\mathrm{trace}(\mathbf{Y}'_{\mathrm{cent}}\mathbf{Y}_{\mathrm{cent}})/(n-1)}$$

(2)

where n is the sample size, p is the number of predictors, and $R^2_{\mathbf{Y}|\mathbf{X}}$ is the sample estimation of the $\rho^2_{\mathbf{Y}|\mathbf{X}}$.

Since fractions of variation represent redundancy statistics, they also need to be adjusted. Fractions [a + b + c], [b + c], and [a + b] can be adjusted directly, leading to [a + b + c]$_{\mathrm{adj}}$, [b + c]$_{\mathrm{adj}}$, and [a + b]$_{\mathrm{adj}}$. The individual fractions [a]$_{\mathrm{adj}}$, [b]$_{\mathrm{adj}}$, [c]$_{\mathrm{adj}}$, and [d]$_{\mathrm{adj}}$ have to be calculated by appropriate subtractions based on [a + b + c]$_{\mathrm{adj}}$, [b + c]$_{\mathrm{adj}}$, and [a + b]$_{\mathrm{adj}}$.

We conducted a Monte Carlo study equivalent to the one used by Kromrey and Hines (1995) who assessed the accuracy of different methods for adjusting sample R^2 in the univariate multiple regression case. The first step was to generate large population matrices (200 000 individ-

uals) with known $\rho^2_{\mathbf{Y}|\mathbf{X}}$ and then draw a large number of samples with replacement from these populations and calculate $R^2_{\mathbf{Y}|\mathbf{X}}$ and $R^2_{(\mathbf{Y}|\mathbf{X})\mathrm{adj}}$ for each sample. We decided to use large generated populations instead of standard protocols such as generating samples using established correlation matrices (see Peres-Neto et al. 2003 for an example) or by defining the ρ^2 as in the method introduced by Cramer (1987). The reason is that these previously used methods are capable of generating population values only for continuous variables; hence we cannot generate species-like data (e.g., abundance) where some sites are occupied (values > 0) and others are not (values = 0).

We started with a real data set comprised of stream fish communities of a watershed in eastern Brazil (Peres-Neto 2004). A total of 27 species and six environmental variables were considered. The first step was to calculate individual slopes between the species and the environmental variables (slopes are presented in Appendix B: Table B1). Slopes were calculated on the centered species and environmental matrices and used as the basis for our simulation study. The next step was to generate a matrix $\mathbf{X}$ containing six random normally distributed variables $\mathcal{N}(0,1)$ with 200 000 observations (rows). The columns of $\mathbf{X}$ were then standardized (i.e., mean = 0 and variance = 1). Then, a data matrix $\mathbf{Y}$ was generated as: $\mathbf{Y} = \mathbf{XB}\mathrm{mlt} + \mathbf{E}$, where $\mathbf{B}$ (Appendix B: Table B1) is a (6 × 27) matrix containing the slopes for each species on each environmental variable; mlt is a multiplication factor used to reduce the slopes so that we can manipulate them to attain the desirable $R^2_{\mathbf{Y}|\mathbf{X}}$ values. The multiplication factor will be given for each simulated population. $\mathbf{E}$ represents a (200 000 × 27) matrix containing $\mathcal{N}(0,1)$ deviates. The last step was to calculate the $\rho^2_{\mathbf{Y}|\mathbf{X}}$ based on the generated $\mathbf{X}$ (200 000 × 6) and $\mathbf{Y}$ (200 000 × 27) matrices. Since all slopes were different from zero, all predictors were active in the sense that they all contributed to the explanation of matrix $\mathbf{Y}$.

Assessing the accuracy of $R^2_{(\mathbf{Y}|\mathbf{X})\mathrm{adj}}$ using a single set of predictors (canonical analysis)

The first set of simulations considered the simplest case of matrices $\mathbf{X}$ and $\mathbf{Y}$ made of continuous data; abundance-like data will be considered later. In the two sets of simulations, we considered the influence of random predictors by manipulating the number of random $\mathcal{N}(0,1)$ variables added to the set of true predictors $\mathbf{X}$, as well as the sample size n. Two populations with $\rho^2_{\mathbf{Y}|\mathbf{X}} = 0.2007$ (mlt = 0.0004) and $\rho^2_{\mathbf{Y}|\mathbf{X}} = 0.6105$ (mlt = 0.001) were considered. In the first set of simulations, 1000 samples of 100 observations each were randomly drawn from the population [$\mathbf{Y},\mathbf{X}$] and a certain number of random $\mathcal{N}(0,1)$ variables were added to the sample $\mathbf{X}$. In the second experiment, 1000 samples with varying numbers of observations were randomly drawn and no random predictors were added to the model. Fig. 2 presents the results of the two
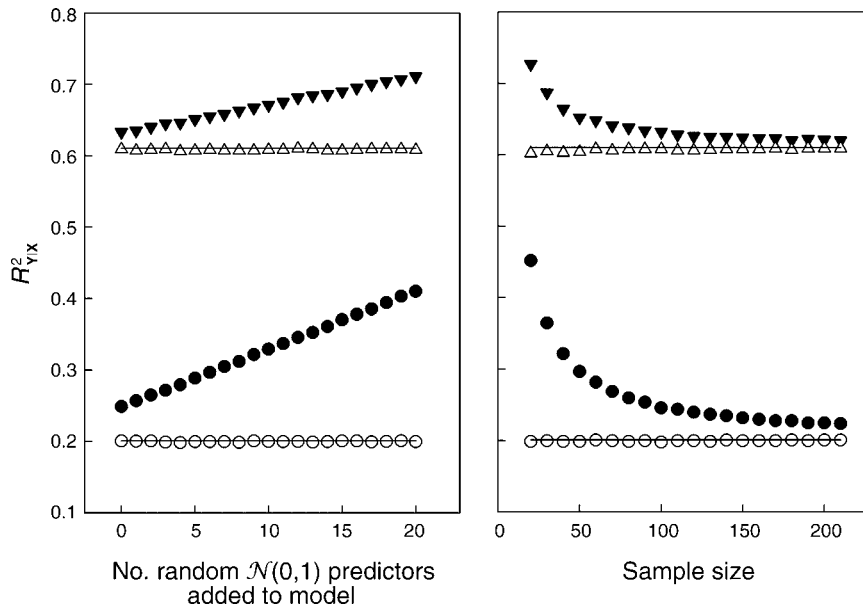
FIG. 2. The influence of null predictors and sample size on the sample mean $R^2_{\mathbf{Y}|\mathbf{X}}$ (solid symbols) and the mean adjusted $R^2_{(\mathbf{Y}|\mathbf{X})\text{adj}}$ (open symbols) considering two RDA populations with normally distributed data. Triangles represent samples from a population $R^2_{\mathbf{Y}|\mathbf{X}} = 0.608$, whereas circles represent samples from a population $R^2_{\mathbf{Y}|\mathbf{X}} = 0.201$. Horizontal lines represent population values. In the case of the influence of the number of null predictors (left panel), samples were based on 100 observations, whereas in the case of the influence of sample size (right panel), no null predictor was added to the model.

simulations; each point in the graphs represents mean values of sample $R^2_{\mathbf{Y}|\mathbf{X}}$ and $R^2_{(\mathbf{Y}|\mathbf{X})\text{adj}}$ based on 1000 random pairs of matrices [**Y**,**X**]. It is evident from these two simulations that the sample $\rho^2_{\mathbf{Y}|\mathbf{X}}$ statistic is highly biased and that $R^2_{(\mathbf{Y}|\mathbf{X})\text{adj}}$ is a much more accurate estimator of the $R^2_{\mathbf{Y}|\mathbf{X}}$. Results (Fig. 2) show that adjusted statistics are always to be preferred to $R^2_{\mathbf{Y}|\mathbf{X}}$ sample values.

Assessing the accuracy of $R^2_{(\mathbf{Y}|\mathbf{X})\text{adj}}$ on variation partitioning (partial canonical analysis)

We conducted a second set of simulations to test whether $R^2_{(\mathbf{Y}|\mathbf{X})\text{adj}}$ also performed well in variation partitioning in canonical analysis involving three data matrices [**Y**,**X**,**W**]. The method used for generating population matrices was basically the same, except that we considered the case where predictors have a certain level of correlation between matrices **X** and **W**. In order to generate populations having predictors **X** and **W** with a given level of correlation (i.e., [b] > 0), the following procedure was applied. (1) Generate a matrix **XW** containing 12 random normally distributed variables $\mathcal{N}(0,1)$ with 200 000 observations. As before, the columns of matrix **XW** were standardized. (2) Generate a (12 × 12) correlation matrix where all cross-correlation values were 0.1. Next, decompose the correlation matrix using Cholesky decomposition. Finally, post-multiply the upper-triangular matrix resulting from the matrix factorization by the matrix **XW** of step 1. (3) The matrix of population slopes $\mathbf{B}_{\mathbf{XW}}$ (12 × 27) is constructed by assembling two slope matrices **B** (6 × 27) (Appendix B:

Table B1). Each one was multiplied by a different multiplication factor, mlt (i.e., $\mathbf{B}_{\mathbf{XW}} = [\mathbf{B}\text{mlt}_{\mathbf{X}}\ \mathbf{B}\text{mlt}_{\mathbf{W}}]$), so that the relative contributions of **X** and **W** to the generated **Y** are different. (4) As before, a data matrix **Y** was generated as: $\mathbf{Y} = \mathbf{XWB}_{\mathbf{XW}} + \mathbf{E}$. The first six columns of matrix **XW** were used to represent matrix **X** and the last six columns became matrix **W**. The population was then represented by juxtaposing the three pertinent matrices as [**Y**,**X**,**W**].

Simulations were also done to evaluate the influence of random predictors and the sample size. Population fractions based on $\text{mlt}_{\mathbf{X}} = 0.0004$ and $\text{mlt}_{\mathbf{W}} = 0.0003$ were as follows: [a + b + c] = 0.3968, [a + b] = 0.3001, [b + c] = 0.2243, [a] = 0.1725, [b] = 0.1276, [c] = 0.0967, and [d] = 0.6032. Matrix **X** contributed to **Y** with a larger portion of the variation in the population (30.01%) than **W** (22.43%), and fraction [b] explained 12.76% of the variation in the population. In the third series of simulations, 1000 samples of 100 observations each were drawn from the population [**Y**,**X**,**W**], and random $\mathcal{N}(0,1)$ variables were added to the sample matrix **W**. In the fourth set of simulations, 1000 samples of a varying numbers of observations were drawn. No random predictors were added to the model. Fig. 3 presents the variation partitioning results from these two last simulations. Each fraction represents mean values of sample fractions and adjusted sample fractions based on the 1000 samples. It is obvious from these results that sample fraction estimates (left panels) are highly biased whereas adjusted fractions (right panels) are much more accurate estimators of the
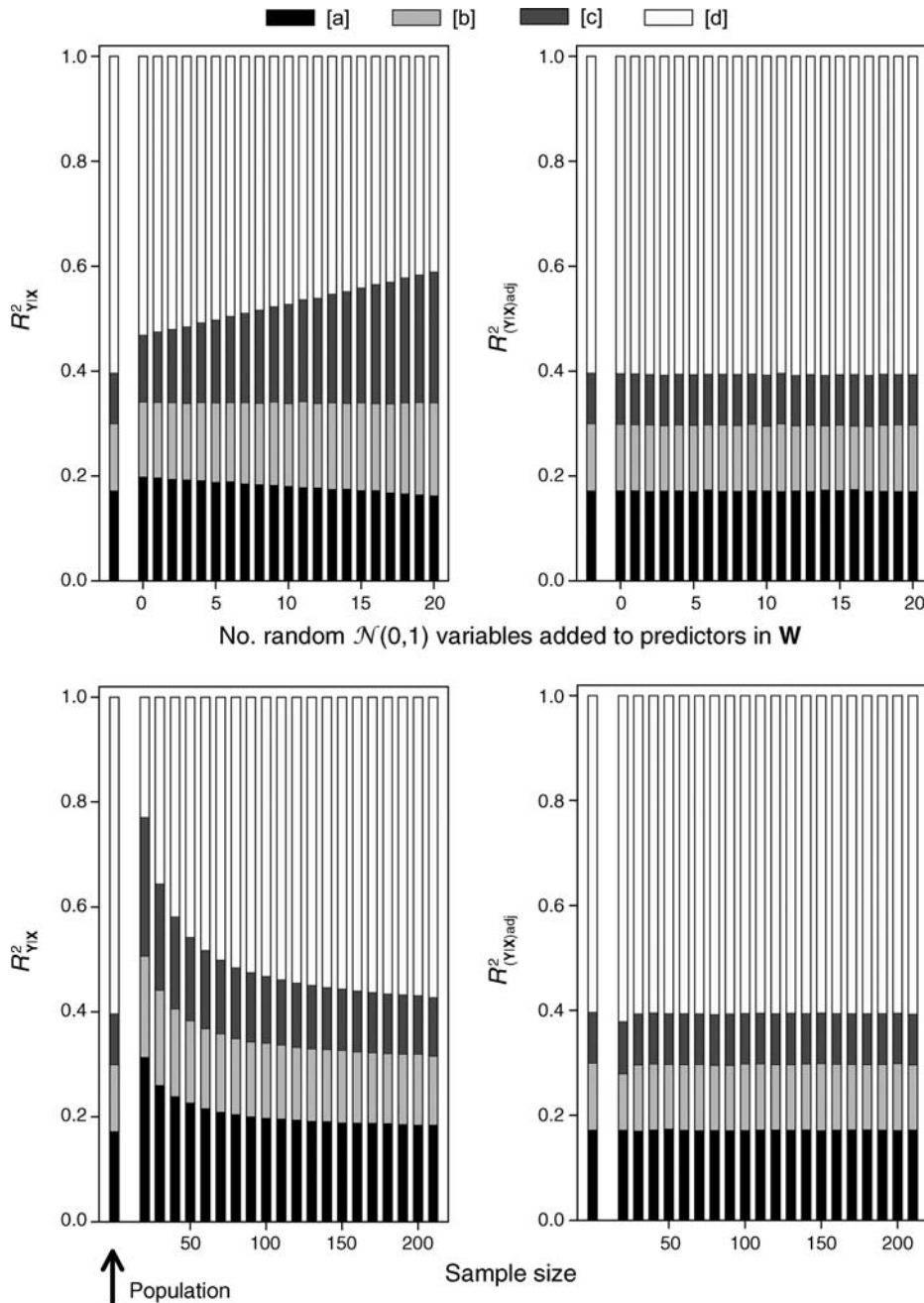
FIG. 3. The influence of null predictors and sample size on fraction estimation in RDA variance partitioning, considering normally distributed data. Left panels, sample $R^2_{Y|X}$; right panels, adjusted $R^2_{(Y|X)adj}$. In the case of the influence of the number of null predictors (upper panels), samples were based on 100 observations, whereas in the case of the influence of sample size (lower panels), only active predictors were used (i.e., no null predictor was added to the model). In that case, all predictors in X were active, whereas in W a mix of active and null predictors was found. The sequence is [a], [b], [c], [d] from bottom to top of each panel.

population values. Although the population fraction [a] is larger than [c], the addition of random variables to matrix W offset the differences in sample fractions without adjustment, demonstrating clearly the need for an adjustment to obtain correct estimates of the importance of each matrix to the model.

ADJUSTED REDUNDANCY STATISTIC FOR THE DISCRETE ABUNDANCE CASE

In the previous section, we considered the case of continuous variables as they represented the case where we expected a direct match between the multiple regression R^2 and the redundancy statistic $R^2_{Y|X}$. How-
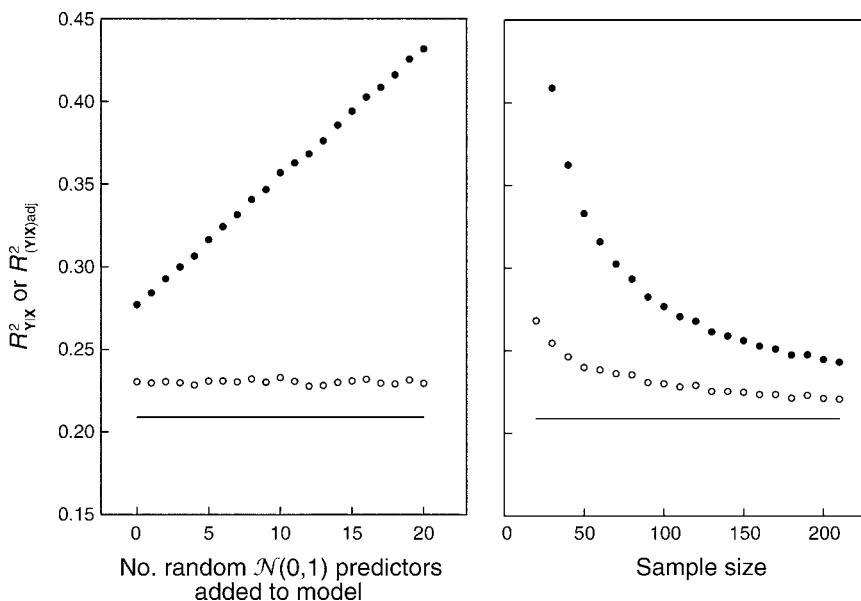
Fig. 4. The influence of null predictors and sample size on the sample mean $R^2_{\mathbf{Y}|\mathbf{X}}$ and the adjusted mean $R^2_{(\mathbf{Y}|\mathbf{X})\text{adj}}$ considering an RDA population ($R^2_{\mathbf{Y}|\mathbf{X}} = 0.2089$) with abundance-like dependent variables. Solid circles represent sample values, and open circles represent adjusted values. Horizontal lines represent population values.

ever, ecologists are most interested in the case where response variables are counts of species abundances, which are discrete and also generally overdispersed and zero inflated (Martin et al. 2005). In order to generate discrete and zero inflated data, we transformed a simulated population matrix $\mathbf{Y}$ as follows: $\mathbf{Y}' = [y'_{ij}] = \exp(1.2(y_{\text{std}ij} - 0.5))$. Once generated, matrix $\mathbf{Y}$ was first standardized into $\mathbf{Y}_{\text{std}}$ so that a variance value of 1.2 could be applied; subtracting 0.5 from the data provided a greater number of zeros (absences; the generated matrices contained roughly 47% zeros). The values y'_{ij} were then rounded to the lower integer to generate $\mathbf{Y}'$. A similar protocol was applied in Legendre et al. (2005). We performed simulations similar to those reported in the previous section, this time using population matrices $\mathbf{Y}'$. We started by investigating the case of RDA. In order to generate $\mathbf{Y}$, a value mlt $= 0.0011$ was necessary to generate a $\rho^2_{\mathbf{Y}|\mathbf{X}} = 0.2089$, which is close to the value generated in the first set of simulations (see *An adjusted redundancy statistic for canonical analysis—the continuous case*). Fig. 4 shows the results as a function of the number of random variables added to sample predictor matrices $\mathbf{X}$ and the sample size. As before, in the case of random predictors, 100 observations were considered. Although the adjusted values provided better estimates than the sample $R^2_{\mathbf{Y}|\mathbf{X}}$, the estimates were quite biased when compared to the $\rho^2_{\mathbf{Y}|\mathbf{X}}$.

Next we investigated the effect of species transformations in the estimates prior to RDA. We used the Hellinger transformation (Legendre and Gallagher 2001) as follows:

$$\mathbf{H} = [h_{ij}] = \left[\sqrt{\frac{y'_{ij}}{\sum\limits_{j=1}^{k} y'_{ij}}} \right] \tag{3}$$

where h_{ij} is the transformed abundance y'_{ij} of species j at site i, and k is the total number of species across all replicates. The use of Hellinger-transformed data prior to performing RDA is equivalent to a distance-based redundancy analysis (db-RDA; Legendre and Anderson 1999) based on Hellinger distance. In the present simulations, the Hellinger-transformed population matrix $\mathbf{H}$ was used instead of $\mathbf{Y}'$. Two Hellinger-transformed population data sets with $\rho^2_{\mathbf{H}|\mathbf{X}} = 0.2071$ (mlt $= 0.0007$) and $\rho^2_{\mathbf{H}|\mathbf{X}} = 0.6099$ (mlt $= 0.0500$) were generated. Contrary to RDA on raw species abundance-like data (Fig. 4), the Hellinger transformation produced much more accurate estimates of $R^2_{\mathbf{H}|\mathbf{X}}$ regarding both sample size and number of random predictors added to the sample matrices (see Appendix C: Fig. C1). The same conclusions were attained when considering variation partitioning as results showed identical patterns as the ones depicted in Fig. 3 for the continuous case (see Appendix C: Fig. C2). Thus, for continuous response variables, Ezekiel's adjustment to RDA R^2 gives quite accurate values, and for the discrete zero inflated data with many zeros (as simulated here), Ezekiel's adjustment using Hellinger-transformed data (i.e., db-RDA on Hellinger distance) is appropriate.
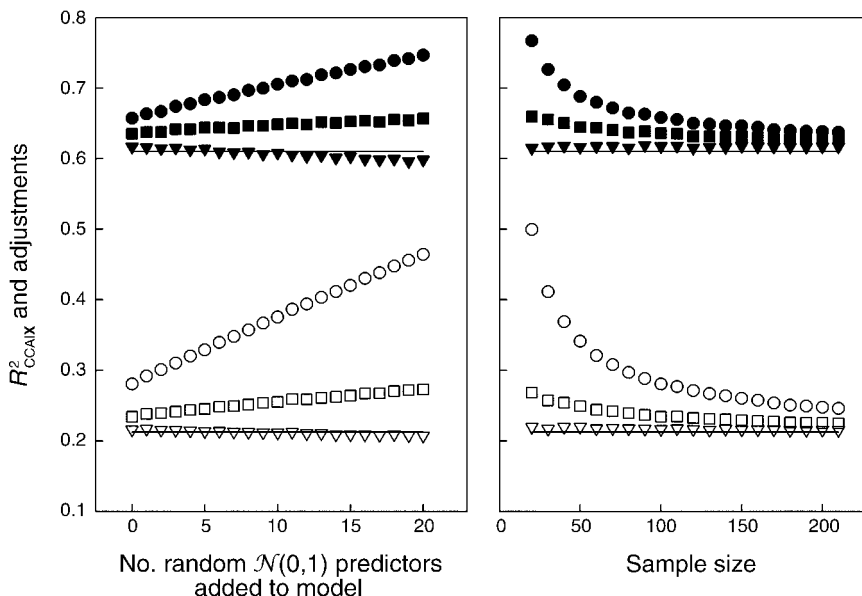
Fig. 5. The influence of null predictors and sample size on the sample mean $R^2_{CCA|X}$ (circles), the mean adjusted R^2_{adj} (squares), and the permutation-based adjusted $R^2_{adj-perm}$ (triangles) considering two CCA populations. Solid symbols in each panel represent samples from a population with $R^2_{CCA|X} = 0.610$, while open symbols represent samples from a population with $R^2_{CCA|X} = 0.213$. Horizontal lines represent population values. In the case of the influence of the number of null predictors (left panels), samples were based on 100 observations, whereas in the case of the influence of sample size (right panels), only active predictors were used (i.e., no null predictor was added to the model).

The Case of CCA and a Permutational Form of Adjustment

Here we present the results of simulations using CCA. As in the two previous sections, we assessed the influence of sample size and number of random predictors added to the model. In the case of random predictors, sample sizes of 100 observations were drawn. Two CCA populations with $\rho^2_{CCA|X} = 0.2128$ (mlt = 0.0011) and $\rho^2_{CCA|X} = 0.6101$ (mlt = 0.0490) were considered. As in the preceding section, values in matrix $\mathbf{Y}$ were transformed into abundance-like values ($\mathbf{Y}'$) after generation and prior to CCA. Ezekiel's adjustments did improve the large bias obtained when using unadjusted R^2 with CCA; however they were still quite inaccurate, especially for the population having $\rho^2_{CCA|X} = 0.2128$ (Fig. 5). We propose a new type of adjustment based on the definition of Ezekiel's formulation. Ezekiel's adjustment is based on the idea that, in regression models, a random predictor explains, on average, under random sampling variation, $1/(n-1)$ of the variation in the response variable. Hence p random predictors explain, on average, under random sampling variation, $p/(n-1)$ of the variation. The adjustment can be rewritten as

$$R^2_{(\mathbf{Y}|\mathbf{X})adj} = 1 - \frac{n-1}{n-p-1}(1 - R^2_{\mathbf{Y}|\mathbf{X}})$$

$$= 1 - \frac{1}{1 - \frac{p}{n-1}}(1 - R^2_{\mathbf{Y}|\mathbf{X}}). \tag{4}$$

Note that when $R^2_{\mathbf{Y}|\mathbf{X}}$ equals $p/(n-1)$, $R^2_{(\mathbf{Y}|\mathbf{X})adj}$ equals zero. In CCA, because a weighted multiple regression is used (see Appendix A), the average $R^2_{CCA|X}$ expected by chance is unknown. We propose that this may be estimated for a given situation using a permutation procedure. The new adjustment hereafter referred to as R^2_{perm} substitutes $p/(n-1)$ in Eq. 4 by an empirical estimate of the value expected under chance alone estimated as follows: (1) randomly permute entire rows of data matrix $\mathbf{X}$ (i.e., no substantial difference was found if regressors were permuted separately), leading to $\mathbf{X}_{perm}$; (2) Calculate $R^2_{CCA|X}$ for a CCA based on $\mathbf{X}_{perm}$; (3) repeat steps 1 and 2 m times (in this study we used $m = 1000$); (4) calculate the mean $\overline{\mathbf{X}}_{perm}$ across all 1000 $R^2_{CCA|X}$ obtained under permutation in step 3. The proposed adjustment is then simply

$$R^2_{perm} = 1 - \frac{1}{1 - \overline{\mathbf{X}}_{perm}}(1 - R^2_{CCA|X}). \tag{5}$$

The correction provides improved estimations in comparison to Ezekiel's adjustment (Fig. 5). The CCA code used here can be used on matrices containing huge number of observations (200 000 observations or more; see Supplement 1 code for CCA) and may be useful for researchers interested in analyzing large data sets.

Testing the Difference between Fractions

Although the adjustment of fractions is an important step toward achieving unbiased canonical models, there

remains the question of whether the influences of two or more groups of predictors (factors), after adjustments, are significantly different. Methods for testing the significance of fractions are well established in the literature as in Legendre and Legendre (1998:608–612). However, one aspect that has not been addressed yet is whether two fractions, say [a] and [c], come from the same statistical population of explained fractions of variation and that they only differ by sampling variation. Such an assessment would provide an important step toward attaining an understanding of the factors patterning community structure. For instance, do environmental factors explain more variation than spatial patterning? In this section, we propose a method for testing for the difference between fractions in canonical variation partitioning. The test proposed here is based on a bootstrap procedure for empirically constructing sampling distributions reflecting the differences between adjusted $R^2_{Y|X}$. The use of bootstrapping as means of adjustment in multiple regressions has been advocated by Kromrey and Hines (1995), but our proposed bootstrap procedure provided a much better estimate than the one proposed by them. The proposed procedure for RDA is as follows.

(1) Compute the RDA residuals based on the original sample for fractions [a + b] and [b + c]:

$$\mathbf{E_X} = \mathbf{Y}_{cent} - \mathbf{XB_X} \qquad \mathbf{E_W} = \mathbf{Y}_{cent} - \mathbf{WB_W} \quad (6)$$

where $\mathbf{E_X}$ and $\mathbf{E_W}$ are $(n \times k)$ matrices of residuals related to the matrix of predictors $\mathbf{X}$ (i.e., [a + b]) and $\mathbf{W}$ (i.e., [b + c]), respectively; n is the number of sites and k is the number of species. $\mathbf{B_X}$ and $\mathbf{B_W}$ are the matrices of slopes for the predictors in $\mathbf{X}$ and $\mathbf{W}$, respectively, and can be calculated simply as: $\mathbf{B_X} = (\mathbf{X'X})^{-1}\mathbf{X'Y}_{cent}$; $\mathbf{B_W} = (\mathbf{W'W})^{-1}\mathbf{W'Y}_{cent}$. Note that $\mathbf{X}$ and $\mathbf{W}$ can be either centered or standardized.

(2) Rescale each column of matrices $\mathbf{E_X}$ and $\mathbf{E_W}$ as

$$\mathbf{E}_{X\text{-scl}} = \sqrt{n/(n - p_X)}\,\mathbf{E_X}$$
$$\mathbf{E}_{W\text{-scl}} = \sqrt{n/(n - p_W)}\,\mathbf{E_W} \quad (7)$$

where p_X and p_W are the number of predictors in matrices $\mathbf{X}$ and $\mathbf{W}$, respectively. Residuals are scaled in this fashion so that the average squared residuals in the bootstrap sample has expectation σ^2 (Wu 1986; i.e., $\mathbf{E} = [e_j] \sim \mathbf{IID}(0, \sigma^2\mathbf{I})$) where $\mathbf{I}$ is a $(n \times 1)$ vector of 1's).

(3) Resample entire rows from the matrix of joint residuals $[\mathbf{E}_{X\text{-scl}}, \mathbf{E}_{W\text{-scl}}]$ with replacement, so that the bootstrapped sample is consistent with the original dimensions of the data matrices leading to $\mathbf{E}_{X\text{-boot}}$ and

$\mathbf{E}_{W\text{-boot}}$. Matrices of residuals were juxtaposed during the bootstrap sampling to make sure that the same rows were randomly chosen in $\mathbf{E}_{X\text{-scl}}$ and $\mathbf{E}_{W\text{-scl}}$, hence maintaining the covariance among predictors in $\mathbf{X}$ and $\mathbf{W}$ during resampling.

(4) Calculate bootstrapped $\mathbf{Y}$ data tables based on matrices $\mathbf{X}$ and $\mathbf{W}$ as the sum of original fitted values plus bootstrapped residuals:

$$\mathbf{Y}_{X\text{-boot}} = \mathbf{XB_X} + \mathbf{E}_{X\text{-boot}}$$
$$\mathbf{Y}_{W\text{-boot}} = \mathbf{WB_W} + \mathbf{E}_{W\text{-boot}}. \quad (8)$$

(5) Calculate fitted values based on the centered values of each set:

$$\hat{\mathbf{Y}}_{X\text{-boot}} = \mathbf{XB_X}(\mathbf{I} - \mathbf{P})\mathbf{Y}_{X\text{-boot}}$$
$$\hat{\mathbf{Y}}_{W\text{-boot}} = \mathbf{WB_W}(\mathbf{I} - \mathbf{P})\mathbf{Y}_{W\text{-boot}}. \quad (9)$$

Bootstrapped adjusted $R^2_{Y|X}$ based on each set of predictors were calculated as shown in Eq. 10 (at bottom of page). $R^2_{(Y|X)\text{adj-boot}^i}$ was calculated in the same way by replacing $\mathbf{Y}_{X\text{-boot}} - \hat{\mathbf{Y}}_{X\text{-boot}}$ by $\mathbf{Y}_{W\text{-boot}} - \hat{\mathbf{Y}}_{W\text{-boot}}$. Note that the total sum of squares (TSS = trace($\mathbf{Y'}_{cent}\mathbf{Y}_{cent}$)) in Eq. 10 was divided by n instead of $(n - 1)$ as in Eq. 2. Our decision was based on the fact that the maximum likelihood estimator of TSS provided better adjusted estimates under bootstrap (see Appendix D).

(6) Repeat steps 3–5 m times ($m = 1000$ in this study). For each bootstrap replicate, calculate the difference between the two adjusted estimates as $D_i = R^2_{(Y|X)\text{adj-boot}^i} - R^2_{(Y|W)\text{adj-boot}^i}$. Then, using all bootstrapped D_i values, build a confidence interval for the differences between adjusted fraction values. There are a number of procedures for estimating confidence intervals (Manly 1997); we used the percentile method (Manly 1997:39). First, D_i values were ordered in ascending order, then we identified the D_i values that occupied the $\alpha m/2$-th and $(1 - \alpha/2)m$-th values in the sorted list, which were then used as confidence limits estimates. Both $\alpha m/2$ and $(1 - \alpha/2)m$ were rounded to the nearest integer. Note that if confidence intervals are reported they can be helpful in comparing differences between fractions based on different data sets (e.g., two or more landscapes). We considered an $\alpha = 0.05$ significance level throughout this study. If the estimated interval did not encompass zero, then the null hypothesis was rejected. Alternatively, a P value can also be estimated. First, calculate the median of D_i values. If the median is positive, then calculate the number of D_i smaller than zero; or alternatively if D_{obs} is negative, calculate the number of D_i larger than zero,

$$R^2_{(Y|X)\text{adj-boot}^i} = [\text{a} + \text{b}]_{\text{adj}_i}$$

$$= 1 - \frac{\text{trace}\Big(\big[(\mathbf{I} - \mathbf{P})\mathbf{Y}_{X\text{-boot}} - \hat{\mathbf{Y}}_{X\text{-boot}}\big]'\big[(\mathbf{I} - \mathbf{P})\mathbf{Y}_{X\text{-boot}} - \hat{\mathbf{Y}}_{X\text{-boot}}\big]\Big)/(n - p_x - 1)}{\text{trace}\big(\mathbf{Y'}_{cent}\mathbf{Y}_{cent}\big)/n} \quad (10)$$
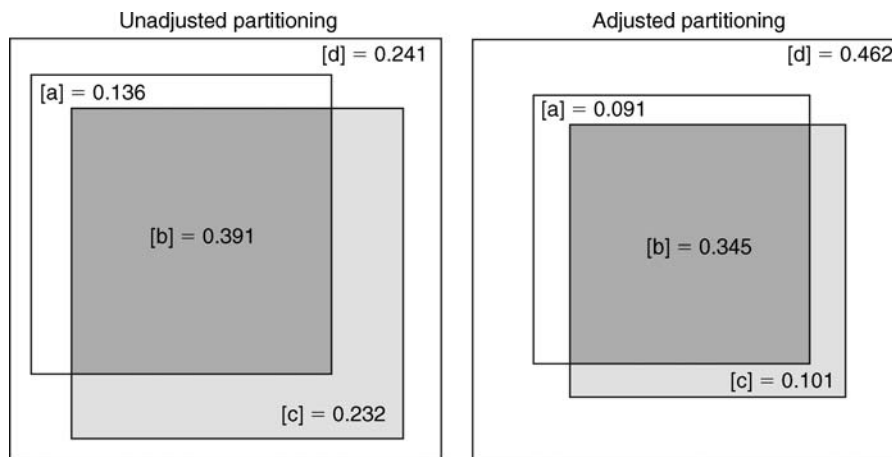
FIG. 6. Variation partitioning Venn diagrams representing the unadjusted (left) and adjusted (right) percentages of unique contribution of [c] spatial and [a] environmental components to the oribatid mite distribution. Fraction [b] represents the shared variation between the environmental and spatial components and [d] the residual variation left unexplained by the canonical model. Distance-based eigenvector maps were used to analyze the spatial component of the mite variation. Although fractions [a] and [c] were both significant in terms of explaining the variation in oribatid mite distribution, the proportions of variation explained by each do not differ significantly from each other (bootstrap test for fractions, $P = 0.4865$).

divided by the number of bootstrap samples, and then multiplied by two in order to make the test two tailed.

In order to assess the statistical robustness of the proposed test, we empirically estimated Type I error rates and power based on Monte Carlo simulations (Peres-Neto and Olden 2001). The complete description of the method involved in this assessment and the detailed results are presented in Appendix E. Type I error rates were either equal to or smaller than the established significance level for both the RDA based on the Hellinger transformation and CCA, hence validating the test (Appendix E).

Variation Partitioning—An Example of Fraction Adjustment and Testing

In this section we present a complete example of the approaches introduced here, where we contrast results based on unadjusted and adjusted fractions in variation partitioning. Data were comprised of the abundances of 35 species of oribatid mites and five habitat variables from 70 soil cores 10×2.6 m in area in the peat blanket surrounding a bog lake originally presented by Borcard et al. (1992). Three of the five environmental variables are qualitative and were transformed into Helmert orthogonal contrasts as used in ANOVA (i.e., each k-level categorical variable was represented by $k - 1$ contrasts). A total of 11 environmental predictors were then used (nine Helmert contrasts representing qualitative variables and two quantitative variables). In order to generate spatial descriptors, we applied a distance-based eigenvector map (Dray et al. 2006) to the spatial coordinates of the cores. Here, the 22 eigenvectors with positive eigenvalues were retained as spatial descriptors to be used in the variation partitioning of the oribatid data. We applied variation partitioning by RDA to the

matrix of Hellinger-transformed data. Results of variation partitioning based on adjusted and unadjusted fractions are presented in Fig. 6. Differences between adjusted and unadjusted fractions were quite noticeable, especially given the large number of spatial descriptors considered and when comparing the residual fraction [d] between the unadjusted and adjusted partitioning. Based on permutation tests (see Legendre and Legendre 1998:608–610), both fractions [a] and [c] explained a significant portion of the variation ($P[a] = 0.001$; $P[c] = 0.001$; 1000 permutations were applied). Based on our bootstrap procedure, however, the spatial and environmental components explained similar proportions of variation ($P = 0.4865$) of the species distribution.

Discussion

Canonical analyses have become standard tools to analyze ecological community data in order to search for patterns and test hypotheses regarding species distributions and structuring factors. Although the issue of adjustment of the explained variation has been greatly stressed in univariate multiple regression modeling, it had not been discussed for canonical analysis applied to ecological data, especially for the case of variation partitioning. The present study brought attention to the importance of adjusting model explanation in canonical analysis and assessed the appropriateness of standard procedures used in regression analysis; it also offered a novel adjustment in the case of CCA. Our study demonstrated that sample $R^2_{Y|X}$ used in canonical analysis and variation partitioning is biased and that adjustments are not only preferable but necessary to provide more accurate estimations and valid comparisons between sets of factors in explaining community structure. Discrepancies between nonadjusted and ad-

justed fractions in variation partitioning will depend on the differences between the numbers of variables in each set of predictors. For instance, spatial regressors are always simpler to generate in comparison to environmental variables. As a result, the spatial fraction could appear more important due to a large number of unimportant spatial predictors considered in the canonical analysis. Indeed, in our example (Fig. 6), we found that the fraction due to the spatial component contributed with almost twice as much variation as the fraction due to the environmental component. Once adjusted, both fractions were quite similar and indeed the bootstrap test of fractions did not detect a significant difference between the environmental and spatial contributions. Adjustments will also permit comparisons between different canonical analyses as they adjust not only for the number of predictors but also for the number of samples. Cottenie (2005), comparing the contribution of environmental and spatial fractions based on 158 published data sets using canonical analysis, was forced to control for the potential bias in the estimation by using subsets of 30 sites and four spatial and environmental predictors in each analysis since appropriate adjustments were not yet available.

Our assessment did not consider the case of presence–absence data, other species transformations (Legendre and Gallagher 2001), and different types of distances such as Bray-Curtis that can be considered in distance-based RDA (Legendre and Anderson 1999). However, the simulation protocols applied here could be easily adapted to assess the accuracy of the adjustments considered here. The permutation approach used in the case of CCA can also be easily implemented in the case of other transformations prior to RDA and to different distances in the case of db-RDA.

The testing procedure for assessing the difference between two fractions of variation in canonical analysis is analogous to the comparison of nonnested models. There is a large body of literature dealing with tests for nonnested models for multiple regressions (Royston and Simpson 1995, Watnik et al. 2001), where sets of predictors are compared. The existing methods for comparing nonnested models, however, determine which set of predictors (model) is the most important in explaining the response variable. In the bootstrap test of fractions proposed here, we consider that the combination of the two sets of regressors is important in explaining the response variable, but that one set may be more important than the other in patterning the response variables (e.g., species). Current implementations for comparing nonnested models may identify whether two sets of predictors are significant or not, but not if the contribution of one set is significantly greater than the other. In addition, these implementations are only applicable to the case of multiple regressors having one response variable and are not implemented for the case of canonical analysis. Overall, we hope that the methods suggested will aid ecologists in attaining an understanding of the factors driving community structure.

A Matlab library and an executable version for conducting variation partitioning based upon adjusted R^2 values in RDA or CCA, and testing fractions, are available in Supplement 2 and Supplement 3, respectively. The R-language function "varpart," available in the vegan library (Version 1.7-81 or higher; Oksanen et al. 2005), automatically conducts variation partitioning of a response table with respect to two, three, or four tables of explanatory variables, using RDA-adjusted R^2 values.

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APPENDIX A

A detailed description of the steps involved in calculation of the redundancy statistics in canonical correspondence analysis (CCA) (*Ecological Archives* E087-158-A1).

APPENDIX B

A table presenting the slopes relating the species to the environmental variables considered in the simulations (*Ecological Archives* E087-158-A2).

APPENDIX C

Results for the Hellinger-transformed species data (*Ecological Archives* E087-158-A3).

APPENDIX D

A simulation study showing the accuracy of the suggested bootstrapped adjusted R^2 (*Ecological Archives* E087-158-A4).

APPENDIX E

Results of simulations to assess the Type I error and power of the proposed bootstrap test of the difference between fractions in variation partitioning, including results for redundancy analysis (RDA) and canonical correspondence analysis (CCA) (*Ecological Archives* E087-158-A5).

SUPPLEMENT 1

Matlab function for conducting canonical correspondence analysis for very large data sets (*Ecological Archives* E087-158-S1).

SUPPLEMENT 2

Matlab library for conducting variation partitioning and test of fractions in multiple regression and canonical models (*Ecological Archives* E087-158-S2).

SUPPLEMENT 3

An executable program for conduction variation partitioning with adjustments, test of fractions in redundancy analysis (RDA) and canonical correspondence analysis (CCA) (*Ecological Archives* E087-158-S3).

Appendices to:

Peres-Neto, P.R., P. Legendre, S. Dray, and D. Borcard. 2006. Variation partitioning of species data matrices: estimation and comparison of fractions. Ecology 87:2614–2625.

<div align="center">

APPENDIX A

***Ecological Archives* E087-158-A1**

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DETAILED DESCRIPTION OF THE STEPS INVOLVED IN CALCULATION OF THE REDUNDANCY
STATISTICS IN CANONICAL CORRESPONDENCE ANALYSIS (CCA)

</div>

1. Transform matrix $\mathbf{Y}$ into a matrix $\overline{\mathbf{Q}}$ of chi-square contributions:

$$\mathbf{P} = [p_{ij}] = [\mathbf{Y}_{ij} / \sum_{i=1}^{n} \sum_{j=1}^{k} \mathbf{Y}_{ij}]$$

$$\overline{\mathbf{Q}} = \mathbf{D}_{1/\sqrt{f_{i+}}} \mathbf{P} \mathbf{D}_{1/\sqrt{f+j}} - \mathbf{D}_{\sqrt{f_{i+}}} \mathbf{1} \mathbf{D}_{\sqrt{f+j}} \tag{1}$$

where $\mathbf{P}$ is a (n x k) matrix of elements p_{ij}. $\mathbf{D}_{1/\sqrt{f_{i+}}}$ is a (n x n) diagonal matrix with

elements $1/\sqrt{f_{i+}}$. f_{i+} is described below; n is the number of sites and k is the number of

species (i.e., number of columns of matrix $\mathbf{Y}$). f_{+j} is the sum of all frequencies

(presence-absence or abundances) f of species j. $\mathbf{D}_{1/\sqrt{f_{+j}}}$ is a (k x k) diagonal matrix

with elements $1/\sqrt{f_{i+}}$. $\mathbf{1}$ is a (n x k) matrix with all elements equal to unity. For

completeness, $\mathbf{D}_{\sqrt{f_{i+}}}$ is a (n x n) diagonal matrix with elements $\sqrt{f_{i+}}$ and $\mathbf{D}_{\sqrt{f_{i+}}}$ is a (n x

n) diagonal matrix with elements $\sqrt{f_{i+}}$. The matrix calculation of $\overline{\mathbf{Q}}$ presented here

gives the same results as equation 9.32 in Legendre and Legendre (1998; p 453).

2. Standardize matrix $\mathbf{X}$ with weights given by the sum of the species frequencies at each

site (i.e., the rows of matrix $\mathbf{Y}$) as follows:

$$\mathbf{X}_{std} = [\mathbf{X}_{ip}] = \left[\cfrac{\mathbf{X}_{ip} - \sum_{i=1}^{n} \mathbf{D}f_{i+}\mathbf{X}_{p} / \sum_{i=1}^{n} f_{i+}}{\sqrt{\cfrac{\sum_{i=1}^{n} \mathbf{D}f_{i+}X_{p}^{2} - (\sum_{i=1}^{n} \mathbf{D}f_{i+}\mathbf{X}_{p})^{2} / \sum_{i=1}^{n} f_{i+}}{\sum_{i=1}^{n} f_{i+}}}} \right] \tag{2}$$

where p the number of regressors, and $\mathbf{D}f_{i+}$ is a (n x n) diagonal matrix with elements

equal to the sum of the rows f_{i+} of the species matrix $\mathbf{Y}$. For instance, the first diagonal

element of this matrix is the sum of all species frequencies (abundances or presence-

absences) f present at site 1. Note that $\sum_{i=1}^{n} f_{i+} = \sum_{i=1}^{n}\sum_{j=1}^{k} Y_{ij}$ (i.e., the sum of all values in

matrix $\mathbf{Y}$) where Y_{ij} is the frequency of species j at site i. In the case of presence-absence

matrices, Y_{ij} is either 1 or 0.

3. Calculate the fitted values for all columns of $\overline{\mathbf{Q}}$ using weighted multiple regression,

instead of the multiple regression used in RDA:

$$\widehat{\mathbf{Q}} = \mathbf{D}_{\sqrt{f_{i+}}}\mathbf{X}_{std}(\mathbf{X}_{std}{}'\mathbf{D}_{f_{i+}}\mathbf{X}_{std})^{-1}\mathbf{X}_{std}{}'\mathbf{D}_{\sqrt{f_{i+}}}\overline{\mathbf{Q}} \tag{3}$$

4. Calculate $R_{Y|X}^{2}$:

$$\mathbf{R}_{\mathbf{Y}|X}^{2} = trace(\widehat{\mathbf{Q}}{}'\widehat{\mathbf{Q}}) / trace(\overline{\mathbf{Q}}{}'\overline{\mathbf{Q}}) \tag{4}$$

or in terms of species weights:

$$R^2_{Y|X} = \sum_{j=1}^{k} \frac{\sum_{i=1}^{n} \overline{\mathbf{Q}}_{ij}^2}{trace(\overline{\mathbf{Q}}'\overline{\mathbf{Q}})} \cdot \frac{\sum_{i=1}^{n} \widehat{\mathbf{Q}}_{ij}^2}{\sum_{i=1}^{n} \overline{\mathbf{Q}}_{ij}^2} \qquad (5)$$

As for RDA (eq. 5 main text), $R^2_{Y|X}$ in CCA also becomes a weighted average of

independent R^2 of individual models (i.e., R^2_j) weighted by the species variance, divided

by the total variance (i.e., $\sum_{i=1}^{n} \overline{\mathbf{Q}}_{ij}^2 / trace(\overline{\mathbf{Q}}'\overline{\mathbf{Q}})$).

APPENDIX B

Ecological Archives **E087-158-A2**

A TABLE PRESENTING THE SLOPES RELATING THE SPECIES TO THE ENVIRONMENTAL

VARIABLES CONSIDERED IN THE SIMULATIONS

TABLE B1. Individual slopes relating the 27 species to the 6 environmental variables considered in the simulations throughout this study.

	Species 1	Species 2	Species 3	Species 4	Species 5	Species 6
Predictor 1	0.662	0.831	0.246	-0.470	-0.161	-0.530
Predictor 2	-0.058	0.022	-0.315	-0.013	-0.247	-0.233
Predictor 3	56.348	20.106	-723.217	-611.426	858.843	-983.626
Predictor 4	56.035	22.099	-723.406	-611.564	859.091	-983.669
Predictor 5	55.597	19.513	-724.010	-611.311	858.307	-983.262
Predictor 6	56.478	20.592	-722.688	-610.936	858.360	-983.391

	Species 7	Species 8	Species 9	Species 10	Species 11	Species 12
Predictor 1	-0.158	-0.581	0.249	-0.952	0.445	0.010
Predictor 2	0.043	0.120	-0.006	0.198	-0.294	-0.229
Predictor 3	625.902	-562.233	-615.060	90.175	208.564	-589.630
Predictor 4	626.807	-562.550	-613.868	89.884	209.552	-588.530
Predictor 5	625.533	-561.534	-614.349	91.327	208.770	-589.006
Predictor 6	625.536	-562.246	-614.050	90.695	209.134	-589.330

	Species 13	Species 14	Species 15	Species 16	Species 17	Species 18
Predictor 1	-0.734	0.540	1.033	0.225	0.522	0.373
Predictor 2	-0.044	-0.169	-0.231	-0.083	-0.423	-0.043
Predictor 3	83.618	-582.083	738.813	196.453	-774.486	598.534
Predictor 4	84.156	-581.295	740.993	195.128	-774.428	599.473
Predictor 5	85.186	-581.814	739.852	195.905	-773.304	600.224
Predictor 6	83.961	-581.782	740.028	195.368	-773.486	599.045

	Species 19	Species 20	Species 21	Species 22	Species 23	Species 24
Predictor 1	-1.270	-0.049	0.788	-0.966	0.123	0.476
Predictor 2	-0.081	-0.135	0.211	0.044	-0.102	-0.236
Predictor 3	-26.611	-142.535	25.803	-1220.003	-8.512	1051.437
Predictor 4	-27.338	-142.657	27.617	-1217.841	-7.279	1053.185
Predictor 5	-25.948	-143.463	27.467	-1218.485	-7.496	1051.579
Predictor 6	-26.698	-143.515	26.568	-1219.019	-8.147	1052.437

Table B1 – continued

	Species 25	Species 26	Species 27
Predictor 1	-0.266	0.853	0.884
Predictor 2	0.010	0.090	-0.523
Predictor 3	-9.037	1240.212	656.884
Predictor 4	-9.214	1240.604	657.273
Predictor 5	-8.376	1239.787	656.591
Predictor 6	-8.904	1239.763	656.530

APPENDIX C

Ecological Archives **E087-158-A3**

RESULTS FOR THE HELLINGER-TRANSFORMED SPECIES DATA
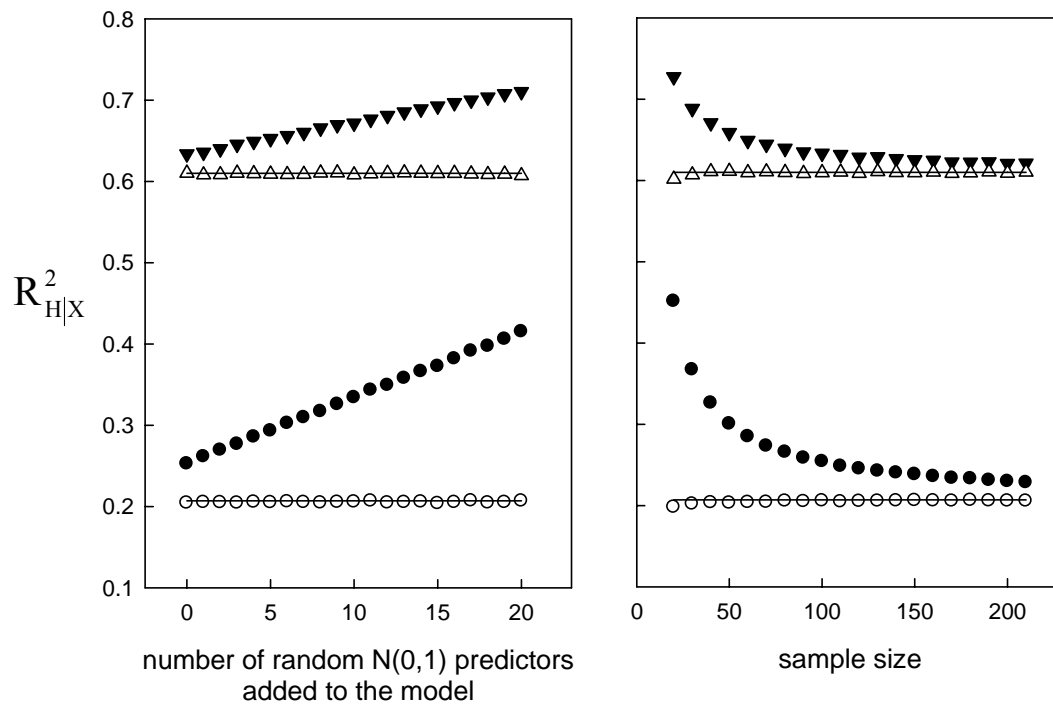
Fig. C1 - The influence of null predictors and sample size on the sample mean $R^2_{H|Y}$ (solid) and the mean adjusted $R^2_{(H|X)adj}$ (open symbols) considering two RDA populations with abundance-like dependent variables that were Hellinger-transformed (see text for explanation). Triangles represent samples from a population with $R^2_{H|Y} = 0.610$ whereas circles represent samples from a population with $R^2_{H|Y} = 0.207$. Horizontal lines represent population values. In the case of the influence of the number of null predictors (left panel), samples were based on 100 observations, whereas in the case of the influence of sample size (right panel), only active predictors were used (i.e., no null predictor was added to the model).
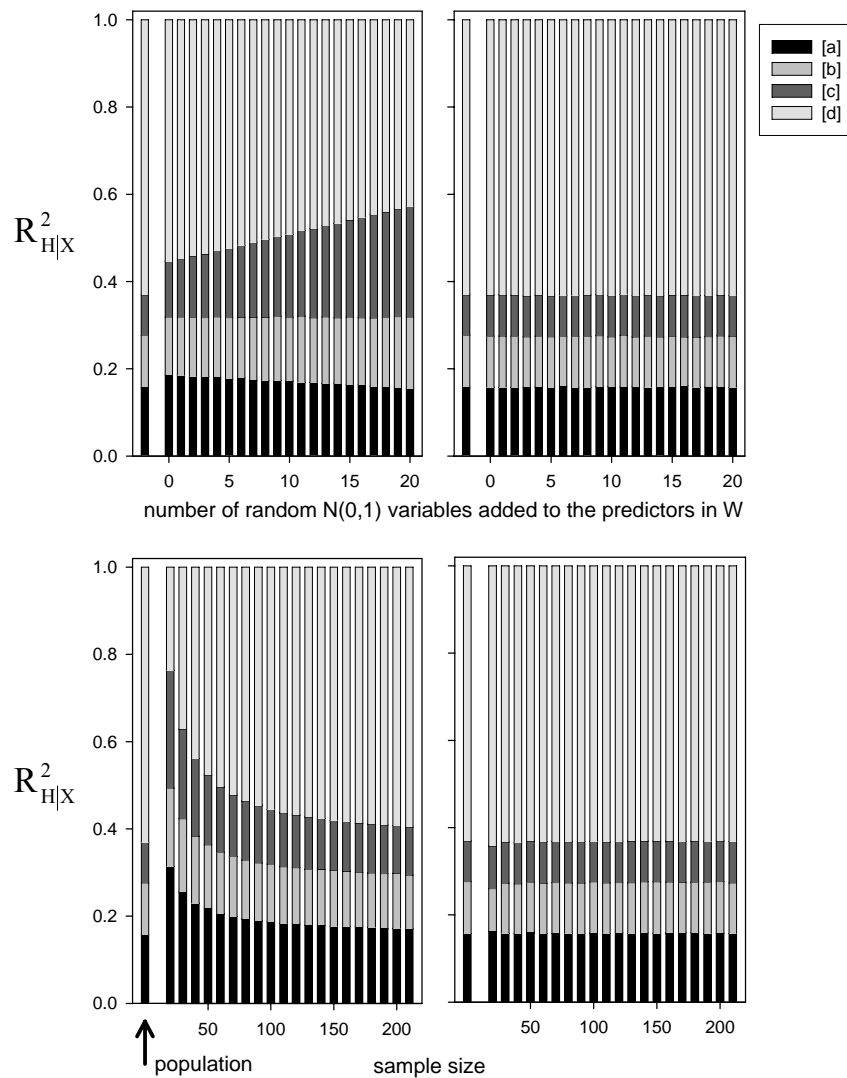
Fig. C2 - he influence of null predictors and sample size on fraction estimation in RDA variance partitioning considering abundance-like dependent variables that were Hellinger-transformed (see text for explanation). Left panels: sample $R^2_{H|X}$; right panels: adjusted $R^2_{(H|X)adj}$. In the case of the influence of the number of null predictors (upper panel), samples were based on 100 observations, whereas in the case of the influence of sample size (lower panel) only active predictors were used (i.e., no null predictor was added to the model). In that case, all predictors in **X** were active, whereas in **W** was found a mix of active and null predictors.

APPENDIX D

Ecological Archives **E087-158-A4**

Simulation study showing the accuracy of the Suggested bootstrapped adjusted R^2:

Bootstrapped adjusted $R^2_{Y|X}$ was calculated as in equation 11, where the total sum-of-squares (SST $= trace(\mathbf{Y}_{cent}'\mathbf{Y}_{cent})$)) in the equation was divided by n instead of $(n-1)$ as in equation 4. Our decision was based on the fact that the maximum likelihood estimator of SST based on n provided better adjusted estimates under bootstrap (Table D2). Here we provide the simulations used to advocate the proposed estimator in equation 11 (text). Simulations were based on multiple regressions (i.e., one response variable) rather than canonical analysis since the only simulation work to assess the accuracy of bootstrap R^2_{adj} used multiple regressions (Ohtani 2000). Another set of simulations, not shown here, indicates that our estimator is also better in the case of canonical analysis. He used a formulation like the one in equation 10, but considering the denominator based on SST$_{Boot}$ ($trace(\mathbf{Y}_{boot}'\mathbf{Y}_{boot})/(n-1)$) instead of

$$trace(\mathbf{Y}_{cent}'\mathbf{Y}_{cent})/n \text{ or } trace(\mathbf{Y}_{cent}'\mathbf{Y}_{cent})/(n-1).$$ He also applied a bootstrap based on residuals, so that results are directly comparable between formulations.

To compare these estimators we applied the protocol implemented in Ohtani (2000) as follows:

1. Generate sample response **y** and predictor **X** variables from ρ^2 (i.e., population R^2) as follows:

$$\lambda = n\rho^2(1-\rho^2)$$

where n is sample size

$$\gamma = \sqrt{\lambda/p}$$

where γ is a (1 x p) vector with all elements equal to $\sqrt{\lambda/p}$

$$\beta = (\mathbf{X'X})^{-0.5}\gamma$$

where β is a (p x 1) vector of slopes, $\mathbf{X}$ is a (n x p) matrix containing p random normally distributed variables N(0,1). Note that columns of $\mathbf{X}$ were standardized (i.e., mean = 0 and variance = 1).

$$\mathbf{y} = \mathbf{X}\beta + \mathbf{e}$$

 where $\mathbf{e}$ represents a (n x 1) vector containing N(0,1) deviates.

2. Generate 1000 samples based on step 1 for a particular combination of ρ^2, n and p and estimate bootstrap adjustments based on 1000 bootstrap samples. Since the ρ^2 (population R^2) is known, we can estimate accuracy by taking the mean over the 1000 estimates of adjusted values and compare it with ρ^2.

3. We considered the same values for ρ^2, the number of predictors and sample size. Table D1 presents the results, indicating that the suggested estimator in equation 1 is the most accurate.

Table D1. Values used in the simulation for comparing bootstrapped adjusted R^2.

p	n	ρ^2	$R^2_{(Y\|X)adj-boot}$ (n)	$R^2_{(Y\|X)adj-boot}$ (n-1)	Ohtani's
3	20	0.9000	0.9044	0.9092	0.9042
		0.6670	0.6699	0.6864	0.6709
		0.5000	0.4994	0.5244	0.5153
		0.3330	0.3337	0.3670	0.3608
	40	0.9000	0.9017	0.9041	0.9029
		0.6670	0.6667	0.6751	0.6662
		0.5000	0.5056	0.5180	0.5060
		0.3330	0.3338	0.3504	0.3450
	80	0.9000	0.9013	0.9025	0.9008
		0.6670	0.6680	0.6722	0.6689
		0.5000	0.5026	0.5088	0.4977
		0.3330	0.3303	0.3387	0.3429
8	20	0.9000	0.9081	0.9127	0.9066
		0.6670	0.6770	0.6932	0.7027
		0.5000	0.5164	0.5406	0.5816
		0.3330	0.3456	0.3783	0.4548
	40	0.9000	0.9034	0.9058	0.9031
		0.6670	0.6714	0.6796	0.6846
		0.5000	0.4997	0.5122	0.5392
		0.3330	0.3350	0.3517	0.3950
	80	0.9000	0.9005	0.9018	0.9021
		0.6670	0.6693	0.6734	0.6751
		0.5000	0.5074	0.5136	0.5217
		0.3330	0.3356	0.3440	0.3703

APPENDIX E

Ecological Archives **E087-158-A5**

RESULTS OF SIMULATIONS TO ASSESS THE TYPE I ERROR AND POWER OF THE PROPOSED

BOOTSTRAP TEST OF THE DIFFERENCE BETWEEN FRACTIONS IN VARIATION PARTITIONING:

AN EXPLANATION AND RESULTS FOR REDUNDANCY ANALYSIS (RDA, TABLES E1 AND E2)

AND CANONICAL CORRESPONDENCE ANALYSIS (CCA, TABLES E3 AND E4)

In order to assess the statistical robustness of the proposed test, we set out to

empirically estimate type I error rates and power based on Monte Carlo experiments

(Peres-Neto and Olden 2001). Type I error rates were estimated by considering

populations where fractions [a] and [c] were equal in values, whereas power was assessed

by creating populations where fractions [a] and [c] had different value. As in our previous

experiments, we considered populations by manipulating the slopes in Table B1 to obtain

the desired fractions. Here, due the computational limitations given the large number of

scenarios considered, instead of building large populations (i.e., $n = 200\,000$), we simply

generated samples with the desired sample sizes. Both procedures are equivalent, but in

the first set of experiments where we wanted to measure the accuracy of the proposed

adjustment, it was necessary to know the exact values of the fractions for the populations.

By setting equal multiplication factors for the slopes used to generate matrices **X**

and **W** (Table B1), we created populations that were suitable for estimating type I error

rates associated with the proposed test, whereas by applying different multiplication

factors we created populations suitable for estimating the power of the test procedure.

Several populations were considered by the combination of multiplication factors and

correlations among predictors to generate desirable [a] and [c] fractions. In addition, in

many scenarios, a certain number of null predictors containing only normal error were

added to either **X** or **W**, or both. We also used a forward selection procedure in order to

assess whether the performance of the testing procedure is increased, especially in the presence of null predictors. The stepwise selection procedure is the same as the permutation-based selection procedure implemented in the program Canoco (ter Braak and Smilauer 2002). 1000 permutations were applied and the selection procedure was stopped when the probability associated with a candidate variable was equal to or smaller than $\alpha = 0.05$. Selection was performed in matrices **X** and **W** separately.

The simulation parameters for each population, the average values across samples for fractions [a], [b] and [c] and rejections rates are presented in Table E1 (type I error) and Table E2 (power). The response variables (species) were Hellinger-transformed. Type I error rates were estimated as the number of times the procedure erroneously reported a significant outcome at the 5% significance level when $mlt_X = mlt_W$. Power was estimated as the number of times a test correctly rejected the null hypothesis at the 5% significance level when $mlt_X \neq mlt_W$). We considered sample sizes of $n = 100$ and 50 observations. In addition, in order to assess the potential influence of the number of species in the test, we considered populations comprised of 27 species (all species of Table B1 were used) and 10 species (only the first 10 species of Table B1 were considered). Estimates were based on 1000 generated sets of data tables. A statistical test is considered valid if the associated type I error rates are not larger than the established level of significance α for any α value. For simplicity, in the case of type I error assessment, we established a fixed confidence interval around the alpha level as 0.036-0.064 (confidence intervals were estimated as: $0.05 \pm \sqrt{0.05(1-0.05)/1000}$ where 0.05 represents α and 1000 is the number of trials). In this way, any estimated type I error rate larger than 0.064 would be considered as significantly different from the expected value of 0.05.

Although type I error rates were not constant across simulations, they were either equal or smaller than the established alpha level when forward selection was not used, hence validating the test (Table E1). While the stepwise procedure was efficient in

eliminating the null predictors present in matrices **X** and **W**, the selected sets of active predictors (i.e., b ≠ 0) were not always consistent across the two matrices of predictors, leading to increased type I error rates (Table E1), especially in the case of samples of 50 observations. Type I error was not affected by considering a smaller number of species.

Power depended consistently on the difference between fractions [a] and [c] and was only slightly affected by the presence of null predictors in the model (Table E2). This was especially the case when only the matrix of predictors having the smallest population fraction contained null predictors, or when both sets of predictors contained null predictors. Since sampling variation of the adjusted fractions may increase in the presence of null predictors, this is also reflected in the bootstrap confidence intervals. This brings attention to the potential use of bootstrap variance as a mean of detecting the presence of null predictors in a data set. When removing a particular predictor, if the bootstrap variance of the statistic $R^2_{(Y|X)adj-boot}$ decreases, this may indicate that the variable in question is either null or contributes to only a small portion of the variation in the model. The power of the test procedure was smaller in the simulations where 10 species only were considered. By analyzing a larger number of species, greater sampling stability was achieved, hence power increased.

It is interesting to note that the estimation of fractions were in average more accurate when using the full set of predictors than when applying forward selection. Rencher and Pun (1980) using simulations found that in univariate multivariate regression, R^2 is in inflated when compared to the expected size. In our case, values were slightly smaller given that before applying the forward selection procedure we conducted an overall test of significance considering all predictors in the model. If the test was not significant, then the forward selection was not conducted and the contribution (R^2) of the set of predictors that was not significant (X or W, or both) was set to 0. Therefore, given the overall test, our results indicate that the selection procedure provides slightly smaller values as opposed to the unrestricted version of Rencher and Pun (1980).

The robustness of the proposed testing procedure was also assessed for CCA.
Note that in this case, CCA residuals were bootstrapped. Simulation parameters and
results are presented in Table E3 (type I error rate) and Table E4 (power). As before,
sample sizes of 100 and 50 observations for populations composed of 27 species, as well
100 observations for populations composed of 10 species, were considered. Forward
selection of predictors was not conducted here, given its lower performance compared to
the direct test of fractions for the Hellinger-based RDA, especially for small sample sizes.
The multiplication factors were modified to obtain measurable differences between the
CCA fractions. Samples based on $mlt_X = 0.0010$ and $mlt_W = 0.0010$ and 10 species
occasionally had 1 or 2 sites per sample without any species present. When this
happened, a species was chosen at random and a value of 1 was placed in the empty row
of matrix **Y** because CCA cannot be computed with species that are missing in all
samples. An important aspect of CCA is the shared fraction [b]. Even if predictors are
perfectly orthogonal (i.e., correlation of zero), fraction [b] in CCA is not 0. This is
because weights based on the species matrix are applied during regression, so that the
predictors are no longer orthogonal after weighting. This analytical aspect could be
modified by weighting the regressors prior to orthogonalization. Note, however, that
current codes (e.g., Canoco, Vegan, PC-ORD) do not carry this implementation since
orthogonal regressors will always provide a non-zero fraction [b] in CCA. Available
computer programs for CCA offer no solution to that problem. As currently implemented,
the analysis of a response data table made of species abundances against factors of an
ecological experiment that were designed to be orthogonal, CCA will not keep the factors
orthogonal and will generate a non-zero fraction [b] representing non-existing shared
explanation of the species abundances data between the orthogonal factors. As in
Hellinger-based RDA (Table E1), type I error rates in CCA (Table E3) were also equal to
or smaller than the established alpha level. Power (Table E4) varied according to the

differences between fractions, and was also smaller when considering populations

consisting of 10 species.

<div align="center">L<small>ITERATURE</small> C<small>ITED</small></div>

Rencher, A.C., and F.C. Pun. 1980. Inflation of R^2 in best subset regression. Technometrics 22: 49-53.

TABLE E1. Type I error rates for the bootstrap-based procedure for testing differences between fractions in RDA variation partitioning, based on the Hellinger-transformed data in matrix **Y**. Estimates are proportions of rejection of the null hypothesis ($\propto = 0.05$) after analyzing 1000 sets of generated data tables. Mlt is the multiplication factor applied to predictor slopes and $r(X,W)$ is the uniform correlation value among predictors. FS stands for forward selection.

| | | | | | | FS | 0.28 | 0.02 | 0.27 | 0.055 | 0.21 | 0.06 | 0.20 | 0.119 | 0.30 | 0.02 | 0.29 | 0.055 |

Mlt for X	Mlt for W	$r(X,W)$	Number of N(0,1) variables added X	Number of N(0,1) variables added W	Selection of variables in model	$n=100$, 27 species Mean estimates [a]	[b]	[c]	Rejection rates	$n=50$, 27 species Mean estimates [a]	[b]	[c]	Rejection rates	$n=100$, 10 species Mean estimates [a]	[b]	[c]	Rejection rates
0.0070	0.0070	0.1	0	0	none	0.14	0.02	0.14	0.022	0.14	0.02	0.14	0.025	0.15	0.03	0.15	0.024
					FS	0.13	0.03	0.13	0.033	0.10	0.04	0.10	0.074	0.14	0.03	0.15	0.040
			5	0	none	0.14	0.02	0.14	0.032	0.14	0.02	0.14	0.015	0.15	0.03	0.15	0.034
					FS	0.13	0.03	0.13	0.031	0.10	0.04	0.10	0.065	0.15	0.03	0.14	0.046
0.1000	0.1000	0.05	0	0	none	0.27	0.12	0.27	0.032	0.27	0.10	0.28	0.057	0.27	0.12	0.27	0.053
					FS	0.27	0.12	0.26	0.043	0.22	0.14	0.23	0.103	0.27	0.13	0.27	0.058
			5	0	none	0.27	0.12	0.27	0.046	0.28	0.10	0.28	0.048	0.28	0.12	0.27	0.048
					FS	0.26	0.13	0.26	0.055	0.23	0.14	0.22	0.104	0.27	0.13	0.26	0.060
			10	0	none	0.27	0.12	0.27	0.052	0.27	0.11	0.28	0.051	0.28	0.11	0.28	0.052
					FS	0.27	0.13	0.26	0.061	0.23	0.16	0.21	0.149	0.27	0.13	0.26	0.061
			5	5	none	0.27	0.12	0.27	0.055	0.27	0.11	0.28	0.056	0.28	0.11	0.28	0.047
					FS	0.26	0.13	0.26	0.068	0.22	0.16	0.22	0.130	0.27	0.13	0.27	0.063
0.0100	0.0100	0.02	0	0	none	0.25	0.04	0.25	0.034	0.25	0.03	0.25	0.048	0.27	0.04	0.27	0.038
					FS	0.24	0.05	0.24	0.039	0.19	0.07	0.19	0.113	0.26	0.05	0.26	0.051
			5	0	none	0.25	0.04	0.25	0.045	0.25	0.03	0.25	0.031	0.27	0.04	0.27	0.041
					FS	0.24	0.05	0.23	0.059	0.19	0.08	0.19	0.112	0.26	0.06	0.25	0.060
0.0008	0.0008	0.02	0	0	none	0.14	0.02	0.14	0.022	0.14	0.02	0.14	0.025	0.15	0.03	0.15	0.024
					FS	0.13	0.03	0.13	0.033	0.10	0.04	0.10	0.074	0.14	0.03	0.15	0.040
			5	0	none	0.14	0.02	0.14	0.032	0.14	0.02	0.14	0.015	0.15	0.03	0.15	0.034
					FS	0.13	0.03	0.13	0.031	0.10	0.04	0.10	0.065	0.15	0.03	0.14	0.046
			10	0	none	0.14	0.02	0.14	0.026	0.14	0.02	0.14	0.019	0.15	0.02	0.15	0.022
					FS	0.13	0.03	0.13	0.035	0.10	0.05	0.10	0.085	0.15	0.03	0.14	0.043
			5	5	none	0.14	0.02	0.14	0.027	0.14	0.02	0.14	0.021	0.15	0.02	0.15	0.022
					FS	0.13	0.03	0.13	0.028	0.10	0.05	0.10	0.076	0.15	0.03	0.15	0.035
0.0200	0.0200	0	0	0	none	0.29	0.00	0.29	0.031	0.29	-0.01	0.30	0.050	0.31	0.00	0.31	0.037
					FS	0.28	0.01	0.27	0.043	0.20	0.06	0.21	0.122	0.29	0.01	0.29	0.056
			5	0	none	0.29	0.00	0.29	0.044	0.30	-0.01	0.29	0.033	0.31	0.00	0.31	0.036

TABLE E2. Power estimates for the bootstrap-based procedure for testing differences between fractions in RDA variance partitioning based on the Hellinger transformed data. Estimates are based on the average proportion of rejections ($\propto$=0.05) per 1000 sample test. Mlt is the multiplication factor applied to predictor slopes and r (X,W) the uniform correlation value among predictors. FS stands for forward selection.

Mlt for X	Mlt for W	r(X,W)	Number of N(0,1) variables added X	Number of N(0,1) variables added W	Selection of variables in model	n=100, 27 species Mean estimates [a]	[b]	[c]	n=100, 27 species Rejection rates	n=50, 27 species Mean estimates [a]	[b]	[c]	n=50, 27 species Rejection rates	n=100, 10 species Mean estimates [a]	[b]	[c]	n=100, 10 species Rejection rates
0.0018	0.0008	0.1	0	0	None	0.23	0.11	0.05	0.995	0.24	0.10	0.05	0.826	0.25	0.12	0.05	0.985
					FS	0.23	0.11	0.04	0.996	0.23	0.10	0.03	0.885	0.26	0.12	0.05	0.987
0.004	0.003	0.1	0	0	none	0.21	0.15	0.12	0.323	0.21	0.14	0.12	0.148	0.22	0.16	0.13	0.295
					FS	0.21	0.15	0.11	0.347	0.19	0.15	0.10	0.232	0.22	0.16	0.12	0.316
0.004	0.003	0.005	0	0	none	0.25	0.08	0.14	0.398	0.25	0.07	0.14	0.183	0.26	0.09	0.15	0.337
					FS	0.24	0.08	0.13	0.444	0.22	0.09	0.10	0.294	0.26	0.09	0.14	0.370
			5	0	none	0.25	0.08	0.14	0.399	0.25	0.07	0.14	0.193	0.26	0.09	0.15	0.344
					FS	0.24	0.09	0.13	0.453	0.22	0.10	0.10	0.310	0.26	0.09	0.14	0.400
			0	5	none	0.25	0.08	0.14	0.378	0.25	0.07	0.14	0.151	0.26	0.09	0.15	0.334
					FS	0.24	0.09	0.13	0.417	0.21	0.10	0.10	0.273	0.26	0.10	0.14	0.358
			5	5	none	0.24	0.08	0.14	0.334	0.24	0.08	0.14	0.152	0.27	0.08	0.15	0.310
					FS	0.24	0.09	0.13	0.408	0.21	0.11	0.10	0.276	0.26	0.09	0.14	0.380
0.04	0.02	0.2	0	0	none	0.25	0.31	0.06	0.748	0.26	0.30	0.07	0.402	0.26	0.33	0.07	0.697
					FS	0.26	0.30	0.06	0.779	0.27	0.29	0.06	0.463	0.27	0.32	0.07	0.717
			5	0	none	0.25	0.31	0.06	0.706	0.26	0.30	0.07	0.401	0.26	0.33	0.07	0.677
					FS	0.26	0.31	0.06	0.775	0.27	0.29	0.06	0.499	0.27	0.32	0.07	0.742
			0	5	none	0.25	0.31	0.06	0.710	0.26	0.30	0.07	0.364	0.26	0.33	0.07	0.665
					FS	0.25	0.31	0.06	0.729	0.26	0.30	0.07	0.435	0.27	0.32	0.07	0.690
			5	5	none	0.25	0.31	0.06	0.678	0.25	0.31	0.06	0.342	0.27	0.32	0.07	0.676
					FS	0.26	0.31	0.06	0.727	0.26	0.31	0.06	0.451	0.27	0.32	0.07	0.728
0.008	0.005	0.05	0	0	none	0.31	0.09	0.12	0.777	0.31	0.08	0.12	0.407	0.33	0.09	0.13	0.709
					FS	0.30	0.09	0.11	0.798	0.28	0.10	0.08	0.530	0.32	0.10	0.12	0.745
0.01	0.005	0.02	0	0	none	0.39	0.03	0.10	0.986	0.39	0.02	0.10	0.771	0.42	0.04	0.10	0.980
					FS	0.37	0.05	0.07	0.990	0.35	0.06	0.05	0.851	0.40	0.06	0.08	0.984
0.015	0.01	0.02	0	0	none	0.36	0.04	0.16	0.698	0.36	0.03	0.16	0.332	0.38	0.04	0.17	0.651
					FS	0.34	0.05	0.14	0.746	0.31	0.07	0.10	0.529	0.36	0.06	0.15	0.717

TABLE E3. Type I error estimates for the bootstrap-based procedure for testing differences between fractions in CCA variance partitioning. Estimates are based on the average proportion of rejections ($\propto$=0.05) per 1000 sample test. Mlt is the multiplication factor applied to predictor slopes and r (X,W) the uniform correlation value among predictors.

Mlt for X	W	r(X,W)	Number of N(0,1) variables added X	W	n=100, 27 species Mean estimates [a]	[b]	[c]	Rejection rates	n = 50, 27 species Mean estimates [a]	[b]	[c]	Rejection rates	n =100,10 species Mean estimates [a]	[b]	[c]	Rejection rates
0.0010	0.0010	0.01	0	0	0.10	0.08	0.10	0.016	0.11	0.08	0.11	0.010	0.12	0.10	0.12	0.015
			5	0	0.10	0.08	0.10	0.009	0.10	0.08	0.11	0.009	0.14	0.09	0.13	0.017
			0	5	0.11	0.08	0.10	0.012	0.11	0.08	0.11	0.003	0.15	0.09	0.13	0.030
			5	5	0.11	0.07	0.11	0.015	0.12	0.06	0.12	0.009	0.14	0.09	0.14	0.016
0.0200	0.0200	0.01	0	0	0.18	0.23	0.17	0.035	0.18	0.22	0.18	0.032	0.20	0.28	0.20	0.033
			5	0	0.19	0.22	0.18	0.037	0.20	0.21	0.19	0.031	0.21	0.27	0.20	0.025
			0	5	0.19	0.22	0.18	0.036	0.20	0.21	0.19	0.033	0.21	0.27	0.20	0.027
			5	5	0.19	0.22	0.18	0.033	0.19	0.21	0.20	0.030	0.21	0.28	0.21	0.034
0.0700	0.0700	0.01	0	0	0.21	0.29	0.21	0.037	0.21	0.28	0.22	0.040	0.21	0.31	0.22	0.037
			5	0	0.22	0.29	0.21	0.035	0.23	0.27	0.23	0.040	0.23	0.31	0.22	0.032
			0	5	0.22	0.29	0.21	0.042	0.23	0.27	0.23	0.039	0.23	0.31	0.22	0.029
			5	5	0.22	0.29	0.21	0.037	0.22	0.27	0.23	0.042	0.22	0.31	0.22	0.037

TABLE E4. Power estimates for the bootstrap-based procedure for testing differences between fractions in CCA variance partitioning. Estimates are based on the average proportion of rejections ($\propto$=0.05) per 1000 sample test. Mlt is the multiplication factor applied to predictor slopes and r (X,W) the uniform correlation value among predictors.

Mlt for			Number of N(0,1) variables added		n =100, 27 species				n = 50, 27 species				n =100,10 species			
					Mean estimates			Rejection rates	Mean estimates			Rejection rates	Mean estimates			Rejection rates
X	W	r (X,W)	X	W	[a]	[b]	[c]		[a]	[b]	[c]		[a]	[b]	[c]	
0.01	0.00	0.01	0	0	0.26	0.11	0.05	0.993	0.27	0.11	0.06	0.827	0.30	0.14	0.06	0.986
			5	0	0.27	0.11	0.06	0.998	0.27	0.11	0.06	0.820	0.32	0.14	0.06	0.998
			0	5	0.26	0.11	0.06	0.978	0.27	0.11	0.06	0.717	0.31	0.14	0.08	0.950
			5	5	0.27	0.11	0.06	0.987	0.28	0.11	0.07	0.755	0.32	0.14	0.07	0.985
0.02	0.01	0.01	0	0	0.32	0.15	0.06	0.995	0.33	0.15	0.07	0.845	0.37	0.20	0.07	0.992
			5	0	0.33	0.15	0.06	0.999	0.34	0.15	0.07	0.858	0.38	0.20	0.07	0.997
			0	5	0.33	0.15	0.07	0.979	0.33	0.15	0.08	0.741	0.38	0.19	0.08	0.971
			5	5	0.33	0.15	0.07	0.994	0.34	0.15	0.07	0.802	0.38	0.20	0.08	0.993
0.04	0.03	0.01	0	0	0.27	0.25	0.13	0.535	0.27	0.24	0.13	0.262	0.29	0.29	0.14	0.496
			5	0	0.28	0.24	0.13	0.570	0.29	0.23	0.14	0.27	0.30	0.28	0.14	0.519
			0	5	0.27	0.24	0.14	0.471	0.28	0.23	0.15	0.204	0.30	0.28	0.15	0.449
			5	5	0.28	0.24	0.14	0.519	0.29	0.23	0.14	0.216	0.30	0.29	0.15	0.478
0.07	0.05	0.01	0	0	0.30	0.27	0.13	0.669	0.31	0.26	0.13	0.340	0.31	0.29	0.13	0.626
			5	0	0.31	0.26	0.13	0.696	0.32	0.25	0.14	0.352	0.33	0.29	0.14	0.638
			0	5	0.31	0.26	0.14	0.610	0.32	0.24	0.15	0.274	0.32	0.29	0.15	0.572
			5	5	0.31	0.27	0.13	0.653	0.32	0.25	0.14	0.284	0.32	0.29	0.14	0.594