Using the right tool for the job: principal component regression and partial least squares regression for analysis of multivariate ecological data.

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# Abstract

# Introduction

Ecologists often want to know which of many possible measured predictor variables are associated with some response. Data collected on many variables for the same individuals presents some unique challenges for data analysis. Multivariate data analysis is not new to the field of ecology, and ecologists have been using techniques like principal component analysis to reduce dimensionality and simplify the interpretation of multivariate data for a long time (Sokal and Rohlf 1995). However, in recent years, the scale of data available for ecological research has increased due to advancements in high-throughput metabolite sampling (Kallenbach et al. 2014; Kfoury et al. 2017), high-throughput phenotyping (Berger et al. 2010; Fahlgren et al. 2015), automated and remote data loggers (Cooke et al. 2004; Porter et al. 2005), remote sensing (Roughgarden et al. 1991; Aplin 2005), high-throughput sequencing technologies (Reuter et al. 2015), and citizen science (Silvertown 2009; Bonney et al. 2009; Dickinson et al. 2012). Simultaneously, there is perhaps and increasing interest in going beyond simply describing multivariate data to inferring processes from patterns. Because multivariate data present problems for linear modeling methods (e.g. multiple regression) (Carrascal et al. 2009), multivariate inference is typically through two general approaches: by reducing dimensionality with unsupervised approaches and conducting hypothesis testing on dimensionally reduced data, or through supervised multivariate analyses.

One typical approach to multivariate statistical inference in ecology is principal component analysis (PCA) followed by a statistical test on the principal component axes generated. PCA creates orthogonal latent variables called principal components that attempt to explain the variation in the predictor variables. Then, the data can be projected onto principal component axes (“scores”) and can be used to look for visual separation or perhaps as predictors in a statistical test for a relationship with some response variable. However, this may not answer the question the researcher is actually asking. Unsupervised techniques like PCA are agnostic to response variables and simply describe the variation in a set of predictor variables. PCA followed by a statistical test on principal components answers the different questions “What are the main axes of variation in the data? Do those axes have a relationship with the response variable?” This approach can be justified when one is truly interested in the axis that describes variation. For example, the leaf economics spectrum (LES) is a highly repeatable principal component that explains variation in leaf traits from a slow to fast rate of return on investments in nutrients and leaf dry matter resulting from a trade-off between metabolic rates and investment to leaf structure (Wright et al. 2004). Because this multivariate trade-off exists across all plants and within groups of plants, it is reasonable to ask questions about how position along the LES varies among habitats, along environmental gradients, or among clades (CITATION). However, a failure to find a relationship with the LES does not mean that measured leaf traits do not vary among habitats, along environmental gradients, or among clades.

Supervised approaches, on the other hand, take response variables into account and test how response variables co-vary with one or more predictor variables. Therefore, a supervised technique answers a fundamentally different question than the unsupervised approach described above. When using a supervised analysis, you are answering the question “Is there a multivariate relationship between the predictors and the response variable?” This may seem a minor distinction, but can lead to completely different conclusions, and unsupervised analyses can even miss statistically significant relationships, as we will demonstrate.

The use of supervised multivariate analyses in ecology may not be as common as… because of some of the challenges ecological data typically creates, including missing values, multicollinearity, small sample sizes, and more variables than observations (AKA the “curse of dimensionality”). Previously, these challenges limited the use of supervised multivariate statistics, but this is no longer the case. In fact, several techniques, including partial least squares regression (PLSR) and its discriminant analysis extension (PLS-DA), handle the above-mentioned challenges of ecological data especially well. Unlike PCA, which creates axes that explain the most variation in the data, PLSR creates axes that explain the most co-variationwith a dependent variable. This is an important distinction because it is not safe to assume that the best explanatory variables will also show the most overall variation among samples.

PLSR was first developed in the late seventies in the field of econometrics (Wold 1975). and later adopted by analytical chemistry (Geladi and Kowalski 1986). In ecology, the use of PLSR has been almost exclusively limited to the sub-field of chemical ecology (Hervé et al. 2018). The underlying assumption of PLSR is that covariation between the predictor variable(s) and the response variable(s) can be explained by a small number of “latent” variables that may or may not be representative of some underlying causal variable. For example, a change in the concentrations of a large number of metabolites may be a result of a change in a single enzyme or metabolic pathway (CITATION). In fact, PLSR has been widely adopted for the analysis of metabolomic data and implemented into many metabolomics-specific statistical software (de Souza et al. 2017). However, the utility of PLSR is not limited to metabolomic data. In fact, one of the strengths of PLSR is that, unlike permutational MANOVA for example, it does not rely on distance or dissimilarity measures and therefore retains information about the relative importance of individual predictor variables (rather than the distance between them). Information about variable importance can be obtained from PLSR axis loadings and variable importance in projection (VIP) scores (CITATION). VIP scores have been shown to be very robust to determining which predictor variables are responsible for variation in the response variable (Chong and Jun 2005). This makes PLSR an ideal technique for highly multivariate ecological datasets where multicollinearity may be present, and the researcher would not only like to address a hypothesis about the effects of some independent variable on a multivariate dataset, but also to determine which measured variables are most responsible for the multivariate relationship.

We demonstrate the use of PLSR and compare it with PCA regression using both a case study approach as well as a simulation study. We then draw on these examples to provide some tips and best practices for implementing PLSR models for ecological data.

# Case Study

Muir et al. (2017) investigated coordination between physiological and morphological leaf traits within a genus in order to understand evolutionary constraints on leaf trait trade-offs. In a common garden experiment, they collected data on leaf traits of 16 *Solanum* species grown from seed. Measured traits included leaf mass per area (LMA), leaf thickness, leaf dry matter content (LDMC), stomatal conductance (*gs*), mesophyll conductance (*gm*), assimilation rate (*A*N), water use efficiency (WUE), maximum rate of carboxylation (*V*cmax) and leaf respiration (*R*dark). In their analysis, Muir et al. performed PCA to recapitulate the leaf economics spectrum (LES)—a highly repeatable principal component axis of leaf traits describing a tradeoff in metabolic rates and investment to leaf structure (Wright et al. 2004). They then used the first principal component (the LES) to answer questions about how the position along the LES varies among habitats and phylogenetic relationships. Here, we reproduce their PCA-based analysis, then use PLSR to answer a different question—do leaf traits vary with mean annual precipitation and temperature of species’ habitats?

### Methods

*Solanum* leaf trait data and coordinates of species habitats are available on Dryad (citation). We used the habitat coordinates to download mean annual precipitation and temperature data from WorldClim (Fick and Hijmans 2017). Muir et al. (2017) identified one species, *S.* *juglandifolium*, as a potential outlier and performed their analyses both with and without that species. For the sake of brevity for this case study, we only performed analyses with this species excluded.

To replicate the approach of the original paper, we performed PCA on leaf traits to recapitulate the LES. Then, the first principal component axis (i.e., the LES) was used as a predictor variable in two regressions with either mean annual temperature or precipitation as response variables.

PLSR was used to test the hypothesis that there is a relationship between climate variables and leaf traits. The two PLSR analyses included all leaf traits as predictor variables and habitat mean temperature or precipitation as response variables. It is possible to include multiple response variables in PLSR models to account for collinearity. However, in this dataset, temperature and precipitation were not correlated (Pearson’s correlation test, r = -0.10, df = 63, p = 0.421) so we chose to perform PLSR for temperature and precipitation separately to improve interpretability. PCA and PLSR were performed using the *opls* function in the *ropls* package in R with default settings other than increasing the number of permutations to 1000 for PLSR (Thévenot et al. 2015).

### Results and Discussion

*Interpretation of PCA regression*

The PCA of leaf traits resulted in two retained principal components with a cumulative R2 of 0.558. The first principal component axis (PC1), which explained 32% of the variation in these data, effectively recapitulated the LES with a strong positive correlation with LMA, LDMC, and leaf thickness and a strong negative correlation with *A*N, *g*m, *V*cmax and *g*s (Table 1). This principal component varies significantly with habitat temperature (F(1,63) = 9.07, p = 0.004) but not with precipitation (F(1,63) = 1.22, p = 0.273). According to Muir et al., the opposite was true when *S. juglandifolium* was included in the data (i.e. precipitation was significant and not temperature), and they concluded that there was limited evidence of leaf trait–climate associations based on these results.

*Interpretation of PLSR*

The PLSR for precipitation produced a model with a single predictive component that explains about 20% of the total variation in the data (Table 2, R2X(cum)) and about 42% of the variation in precipitation (Table 2, R2Y(cum)). Q2 is astatistic generated by internal cross-validation that can indicate overfitting or poor predictive power of a model (Eriksson et al. 2006). Q2 is always lower than R2Y, but when it is much lower, it indicates overfitting. In this case, Both R2Y and Q2 are relatively low but similar indicating moderate explanatory and predictive power, but a lack of overfitting. The significance of the model is determined by permutation and re-calculation of the R2Y and Q2 values. The p-values for R2Y and Q2 both indicate there is a highly significant, moderately strong, relationship between precipitation and leaf traits.

For precipitation, the VIP scores and loadings show that LMA, LDMC, and leaf thickness are positively correlated with precipitation (Table 1). Plants living in wet climates have thicker, denser leaves compared to those living in dry climates. The loadings for the precipitation PLSR are similar to those for the first principal component, but without the strong tradeoffs with measures of photosynthetic capacity that are part of the LES. The lack of statistical significance in the PCA regression for precipitation is likely because photosynthetic traits are strongly loaded on PC1 and don’t actually vary with precipitation.

The PLSR for temperature also produced a highly significant single component model with similar explanatory (R2Y) and predictive (Q2) power to the precipitation PLSR. VIP scores and predictive component loadings indicate a negative relationship between temperature and *V*cmax, *A*N, WUE, *R*dark and leaf thickness and a positive relationship with LDMC. Unlike the first principal component, physical leaf traits are not correlated on this predictive axis and there is a positive relationship between temperature and LDMC, but a slight negative relationship with thickness. Plants living in hotter climates therefore have more dense and thin leaves compared to plants from cooler climates.

Comparison of PCA regression to PLS regression

If our question of interest is “are there leaf trait–climate associations?”, then PLSR is an appropriate approach that tells us there is a small, but highly significant relationship between leaf traits and both precipitation and temperature. The main axis of co-variation with temperature is quite different from that with precipitation and neither are very similar to the main axis of overall variation (i.e. PC1). These differences are not surprising given that PCA is agnostic to habitat variables (temperature, precipitation) while PLSR is explicitly attempting to explain co-variation with habitat variables.

Table 1. Loadings from the first two principal components from PCA (PC1, PC2) and the first predictive component from PLSR (P1). VIP scores greater than 1 indicate the importance of a variable in the PLSR model.



Table 2. Model diagnostics from PLSR for both precipitation and temperature.



# Simulated data

### Methods

To further demonstrate some of the properties of PLS and PCA, we used randomly generated multivariate data created with different covariance structures. All multivariate datasets had 20 observations, one factor with two levels (10 observations per level), and 25 continuous variables. All 25 variables had a variance of 1 and a mean of 0 when they were not discriminating between factor levels. Covariance and the difference in means between factor levels was adjusted depending on the scenario:

1) “Null”: 5 variables with covariance of 0, and two groups of 10 variables with a covariance of 0.5 (Fig 1A).

2) “Needle in a haystack”: two groups of 10 variables with covariance of 0.5 and 5 variables with a difference in means of 2 (Fig 1D).

3) “Control” where two sets of 5 variables covary moderately with covariance = 0.5 and discriminate between groups (difference in means = 2); 5 variables with covariance = 0.5 and no difference in means; and 10 variables that do not covary or distinguish groups (i.e. noise) (Fig 1G).

Multivariate data were simulated in R using the *holodeck* package (Scott 2019), which allows simple generation of multivariate data frames with varying correlation structures. We created 100 randomly generated datasets using the same parameters under each of these scenarios.

PCA discriminant analysis (PCA-DA) was performed by first fitting a PCA using the *opls* function from the *ropls* package, which selects a number of principal components using an autofit criterion (Thévenot et al. 2015). Then a linear regression was performed using all retained principal components as predictor variables and a p-value from a global F test is reported.

PLS-DA was conducted using the *opls* function from the *ropls* package with default settings except increasing the number of permutations to 500 to calculate p-values (Thévenot et al. 2015).

For both PCA-DA and PLS-DA, root mean squared error of prediction (RMSEP) was calculated by external 7-fold cross-validation with the help of the *rsample* package (Kuhn and Wickham 2019).

We were also interested in the ability of PCA-DA and PLS-DA to identify important discriminating variables in the “control” and “needle in a haystack” scenarios. To test this, we set criteria for both methods (PCA and PLS-DA) to identify important discriminating variables. For PCA-DA, a variable was considered important if had a significant Pearson correlation (p < 0.05) with any of the principal components that had a significant relationship with the response variable. Two separate criteria were used to determine important variables from PLS-DA models. First, variables were selected as important if they had significant correlations to the predictive axes retained in the PLS-DA models, similar to the criteria used for PCA-DA above. In the second method, a variable was selected if it had a variable importance in projection (VIP) score greater than 1—a common criterion used for variable selection in PLS-DA (Chong and Jun 2005). For each model, each variable was categorized as important or not. We then compared these values to known variable identities (generated as discriminating or not) and created a confusion matrix for each dataset with the number of discriminating variables correctly identified as important being a true positive. From this, we calculated a Cohen’s kappa for each dataset, which describes the accuracy of the method for choosing discriminating variable (Cohen 1960). A kappa of 1 indicates complete accuracy while a kappa of 0 indicates important variables are selected no better than by chance. A negative kappa indicates that selection of important variables is worse than chance. Cohen’s kappa was calculated using the *psych* package for R (Revelle 2018).

See supplemental files for reproducible R scripts.

### Results and Discussion

Under the null scenario, both PCA-DA and PLS-DA are expected to find no separation between groups. Due to a lack of convergence, 3 of the PCA-DA models failed. The remaining 97 models explained about 55% of the variation in the predictor variables on average (R2X, table 3) and the resulting PCs explain about 15% of the variation in the response variable (R2Y, Table 3). The mean p-value from the PCA-DA models is high (p = 0.463), and there is a clear lack of separation in the score plot (Fig 1B). For PLS-DA, 75 out of 100 models failed because the first predictive component was not significant (Thévenot et al. 2015). The 25 PLS-DA models that were successfully built have low R2Y and Q2 values, which is an indicator of poor model performance (Table 3). When a 1 component model is forced, the mean Q2 value is negative, indicating very poor model performance. Even in such models with poor predictive power and non-significant p-values, some separation in the PLS-DA score plot can be observed (Fig 1C). This is a feature of PLSR because some predictor variables will be associated with the response by chance, and this chance of spurious separation increases with the number of variables. Therefore, it’s not generally recommended to show or interpret score plots for non-significant models, and we’ve only included such a plot for heuristic purposes.

Under the control scenario, both PCA-DA and PLS-DA are expected to find significant separation between groups. the PCA-DA for two of the datasets failed due to lack of convergence. PCA-DA explains about 56% of the variation in the predictor variables (R2X) and the PCs explain about 80% of the variation in the response variable (R2Y, Table 3). The p-values obtained from the regression portion of the PCA-DA model are highly significant (p<0.001). The mean R2Y value for PLS-DA models is slightly higher than for PCA-DA (83.5%), but the R2X is much lower (31%). This is expected since PCA attempts to explain variation in the predictor variables and PLS-DA is only attempting to explain co-variation with the response variable. For PLS-DA, mean Q2 is also high, and permutation testing is highly significant (pQ2 = 0.002 ± 0.001), indicating a strong and highly significant relationship between the response and predictors. Although both PCA-DA and PLS-DA give highly significant p-values, PLS-DA has a lower RMSEP indicating less overfitting. Because the discriminating variables are also the variables that contribute the most to overall covariation in the dataset, PCA-DA and PLS-DA are nearly equivalent, despite answering slightly different questions. Here, PCA-DA is answering the question “Is there a main axis of variation in the data?” and then “does that axis explain differences between groups?” PLS-DA, on the other hand, is answering the question “What variables (if any) explain the difference between groups?”

For the needle in a haystack scenario, we would expect PCA-DA to find principal components that do not explain differences between groups, since the variables that distinguish groups do not co-vary strongly. Indeed, PCA-DA models were built for 97 models (3 failed due to convergence errors) and have a mean R2X similar to the control scenario (Table 3). However, R2Y is lower compared to the control scenario and the relationship between the PCs and the response variable is not statistically significant on average (mean p = 0.106). PLS-DA, on the other hand, explains less variation in the predictor variables (R2X), but nearly 91% of the variation in the response variable despite only 5 out of 25 variables having been generated with different means in the two groups. Q2 is high, indicating good model performance, and both pR2Y and pQ2 are highly significant (Table 3). Additionally, the RMSEP is lowest for PLS-DA and similar to the RMSEP for PLS-DA in the control scenario indicating that PLS-DA does just as well when there are only 5 discriminating variables as when there are 10.

Table 3. Model statistics from simulation study. For each statistic a mean ± standard deviation is reported calculated from n models. For PCA-DA and PLS-DA the number of components was determined by the opls function, and in the case of the null scenario the best number of components was zero, in which case a model wasn’t built. For PLS-DA (ncomp forced), a one or two component model was forced.



A close up of a map

Description automatically generated

Figure 1: Multivariate analysis of representative datasets from three data scenarios: “null” (A, B, C), “control” (D, E, F) and “needle in a haystack” (G, H, I). The first column shows correlation heatmaps (A, D, G). Variable names on the axes that begin with “C” were generated with a covariance of 0. 5, those that begin with “N” were generated with a covariance of 0, and those that begin with “D” were generated to have different means in the two groups. The second column shows PCA score plots (B, E, H). The third column shows PLS-DA plots (C, F, I). For PLS-DA plots, the first two predictive axes are plotted, Q2 values are calculated using 7-fold cross validation, and pQ2 is calculated with 500 permutations (C, F, I). Ellipses represent 95% confidence bounds, parenthetical numbers on axis labels are the percent of total variation explained by the axis. Note that in C, the PLS-DA is clearly not a good model due to low Q2 value. We recommend not including a such PLS-DA score plot for non-significant results in a publication.

*PLS-DA identifies discriminating variables while PCA identifies variables with high variation.* PLS-DA identifies variables that were created with different means in the two levels of our factor better than PCA-DA (Fig 2). Under the control scenario, values of kappa were always greater than 0 for PCA-DA and both variable selection methods for PLS-DA. However, even in the control scenario where PCA-DA and PLS-DA performed similarly in finding separation between groups, PLS-DA outperforms PCA-DA at correctly identifying the variables most responsible for that separation, especially when using VIP scores (Fig 2A). Under the needle in a haystack scenario, the difference between PCA-DA and PLS-DA is more dramatic. Kappa values for PCA-DA are lower and more variable among datasets compared to kappa values for both PLS-DA methods.

A close up of a map

Description automatically generated

Figure 2. Kernel density estimate of the distribution of Cohen’s kappa for the control (A) and needle in a haystack (B) scenarios for PCA-DA (red, solid line) and PLS-DA using two importance criteria: correlation with predictive axes (green, dashed line) and VIP > 1 (blue, dotted line). A kappa value of 1 means perfect identification of discriminating variables by the model while a value of zero indicates the model performed no better than random chance.

# Conclusion

With multivariate data analysis, it is important to think about the question you are trying to answer. If you are primarily interested in predictor variables that vary among individuals or observations, then PCA regression might be the most appropriate technique. However, if you are looking for the predictors that best explain a response variable, a supervised approach like PLSR is more appropriate. From very early on in the adoption of PCA regression in ecology, it was suggested that this method might miss important relationships with a response variable, but only in the case when “nature is downright mean” (Jolliffe 1982). We have shown in a case study that nature can be downright mean—that is, reducing dimensionality with an unsupervised approach like PCA can obscure important relationships with response variables. It is not unreasonable to expect situations in nature where the best predictors of a response variable are not the predictors that (co)vary the most among all observations. Advances in statistical techniques and high-power computing mean there is no need to rely on the benevolence of nature and hope your important variables aren’t buried in a principal component analysis. Instead, PLSR and many other supervised approaches are available for testing multivariate hypotheses.

Guidelines for using and reporting results from PLS(DA).

While our work in this paper uses only one of many implementations of PLS regression, the same general guidelines can be generalized to the use of PLS regression and reporting of results using any statistical package. First, because PLS regression focuses on co-variation between predictors and response, it’s possible for a statistically significant relationship to be due to a small number of predictor variables (as in our needle in a haystack scenario) The proportion of variation in the predictors and the number of important variables should be taken into account when interpreting and reporting results. Second, because PLS is prone to overfitting, cross-validation of some sort is necessary to determine model predictive power. When cross-validation indicates a weak model (a low Q2 value, for example), this should also be taken into account when interpreting results. Third, it is important to remember that score plots for PLS models differ from PCA because the predictive axes of PLS models are built to maximize co-variation with the response variable. This means that even statistically non-significant models may show some visual separation in score plots. Because physical distance between points has little meaning in a PLS-DA score plot, we recommend that score plots be used sparingly for PLS-DA. However, in the case that there are more than two groups, or if a score plot is displayed alongside a loading plot, they may be useful visuals. We recommend being explicit about interpretation of model strength and significance using appropriate statistics (e.g. Q2 and p-values) rather than visual separation in score plot figure captions. The nature of PLS score plots also means that unlike PCA regression or PCA-DA, it is entirely inappropriate to base statistical significance of a PLS model on any statistical test of predictive axis scores. Instead, permutation testing can be used to assess statistical significance of model quality statistics such as R2Y or Q2 values. Finally, variable selection can be used to identify which predictors best explain variation in the response. This can be done with VIP scores, which [SENTENCE ABOUT WHAT VIP SCORES DO]. It is important to note that the cutoff of VIP > 1 is somewhat arbitrary and may require adjustment based on properties of particular datasets. Additionally, if you expect many predictor variables to be unrelated to the response, a different approach using sparse PLS (sPLS) might be valuable. Sparse PLS-DA (sPLS-DA) performs variable selection and classification together rather than using VIP scores post-hoc to determine important predictors (Lê Cao et al. 2011).

* Mention extensions to PLS like orthogonal (OPLS) and sparse (sPLS) versions. Also time series PLS and I guess PLS with interactions is also possible, but I don’t know if it’s in software yet.
* Mention other supervised multivariate analyses like RDA (and cite Herve et al)
* Suggest other ecological questions where PLS might be helpful (cite examples)

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