VEGAN: AN INTRODUCTION TO ORDINATION

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Vegan is a package for community ecologists. This documents explains how the commonly used ordination methods can be done in vegan. The document only is a very basic introduction. Another document (vegan tutorial) (http://cc.oulu.fi/~jarioksa/opetus/method/vegantutor.pdf) gives a longer and more detailed introduction to ordination. The current document only describes a small part of all vegan functions. For most functions, the canonical references are the vegan help pages, and some of the most important additional functions are listed at this document.

1. Ordination

The vegan package contains all common ordination methods: Principal component analysis (function rda, or prcomp in the base R), correspondence analysis (cca), detrended correspondence analysis (decorana) and a wrapper for non-metric multidimensional scaling (metaMDS). Functions rda and cca mainly are designed for constrained ordination, and will be discussed later. In this chapter I describe functions decorana and metaMDS.

- 1.1. **Detrended correspondence analysis.** Detrended correspondence analysis (DCA) is done like this:
- > library(vegan)
- > data(dune)
- > ord <- decorana(dune)

This saves ordination results in ord:

> ord

Date: Id: intro-vegan. Rnw 1260 2010-08-17 12:11:04Z jarioksa processed with vegan 1.17-12 in R version 2.13.0 (2011-04-13) on August 17, 2011.

```
Call:
```

decorana(veg = dune)

Detrended correspondence analysis with 26 segments. Rescaling of axes with 4 iterations.

DCA1 DCA2 DCA3 DCA4
Eigenvalues 0.5117 0.3036 0.12125 0.14266
Decorana values 0.5360 0.2869 0.08136 0.04814
Axis lengths 3.7004 3.1166 1.30057 1.47883

The display of results is very brief: only eigenvalues and used options are listed. Actual ordination results are not shown, but you can see them with command summary(ord), or extract the scores with command scores. The plot function also automatically knows how to access the scores.

1.2. Non-metric multidimensional scaling. Function metaMDS is a bit special case. The actual ordination is performed by function isoMDS of the MASS package. Function metaMDS is a wrapper to perform non-metric multidimensional scaling (NMDS) like recommended in community ordination: it uses adequate dissimilarity measures (function vegdist), then it runs NMDS several times with random starting configurations, compares results (function procrustes), and stops after finding twice a similar minimum stress solution. Finally it scales and rotates the solution, and adds species scores to the configuration as weighted averages (function wascores):

```
> ord <- metaMDS(dune)</pre>
Run 0 stress 12.05894
Run 1 stress 19.48167
Run 2 stress 18.91768
Run 3 stress 12.04546
... New best solution
... procrustes: rmse 0.003150517 max resid 0.01081471
Run 4 stress 11.97273
... New best solution
... procrustes: rmse 0.01994368 max resid 0.0628057
Run 5 stress 11.97273
... New best solution
... procrustes: rmse 4.255425e-05 max resid 0.0001047147
*** Solution reached
> ord
Call:
metaMDS(comm = dune)
Nonmetric Multidimensional Scaling using isoMDS (MASS package)
Data:
          dune
Distance: bray
Dimensions: 2
Stress:
           11.97273
Two convergent solutions found after 5 tries
Scaling: centring, PC rotation, halfchange scaling
```

Species: expanded scores based on 'dune'

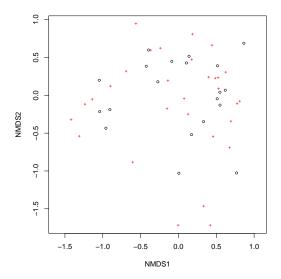


FIGURE 1. Default ordination plot.

2. Ordination graphics

Ordination is nothing but a way of drawing graphs, and it is best to inspect ordinations only graphically (which also implies that they should not be taken too seriously).

All ordination results of vegan can be displayed with a plot command (Fig. 1): > plot(ord)

Default plot command uses either black circles for sites and red pluses for species, or black and red text for sites and species, resp. The choices depend on the number of items in the plot and ordination method. You can override the default choice by setting type = "p" for points, or type = "t" for text. For a better control of ordination graphics you can first draw an empty plot (type = "n") and then add species and sites separately using points or text functions. In this way you can combine points and text, and you can select colours and character sizes freely (Fig. 2):

```
> plot(ord, type = "n")
> points(ord, display = "sites", cex = 0.8, pch = 21, col = "red",
+     bg = "yellow")
> text(ord, display = "spec", cex = 0.7, col = "blue")
```

All vegan ordination methods have a specific plot function. In addition, vegan has an alternative plotting function ordiplot that also knows many non-vegan ordination methods, such as prcomp, cmdscale and isoMDS. All vegan plot functions return invisibly an ordiplot object, so that you can use ordiplot support functions with the results (points, text, identify).

Function ordirgl (requires rgl package) provides dynamic three-dimensional graphics that can be spun around or zoomed into with your mouse. Function ordiplot3d (requires package scatterplot3d) displays simple three-dimensional scatterplots.

2.1. Cluttered plots. Ordination plots are often congested: there is a large number of sites and species, and it may be impossible to display all clearly. In particular, two or more species may have identical scores and are plotted over each other. Vegan does not have (yet?) automatic tools for clean plotting in these cases, but here some methods you can try:

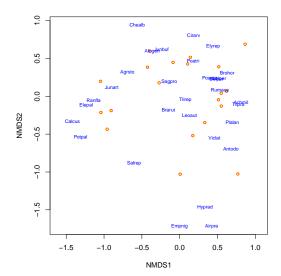


FIGURE 2. A more colourful ordination plot where sites are points, and species are text.

- Zoom into graph setting axis limits xlim and ylim. You must typically set both, because vegan will maintain equal aspect ratio of axes.
- Use points and label only some of these with identify command.
- Use select argument in ordination text and points functions to only show the specified items.
- Use ordilabel function that uses opaque background to the text: some text labels will be covered, but the uppermost are readable.
- Use automatic orditorp function that uses text only if this can be done without overwriting previous labels, but points in other cases.
- Use automatic ordipointlabel function that uses both points and text labels, and tries to optimize the location of the text to avoid overwriting.
- Use interactive orditkplot function that draws both points and labels for ordination scores, and allows you to drag labels to better positions. You can export the results of the edited graph to encapsulated postscript, pdf, png or jpeg files, or copy directly to encapsulated postscript, or return the edited positions to R for further processing.
- 2.2. Adding items to ordination plots. Vegan has a group of functions for adding information about classification or grouping of points onto ordination diagrams. Function ordinal adds convex hulls, ordiellipse adds ellipses of standard deviation, standard error or confidence areas, and ordispider combines items to their centroid (Fig. 3):

In addition, you can overlay a cluster dendrogram from hclust using ordicluster or a minimum spanning tree from spantree with its lines function. Segmented arrows can be added with ordiarrows, lines with ordisegments and regular grids with ordigrid.

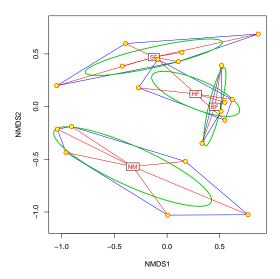


FIGURE 3. Convex hull, standard error ellipse and a spider web diagram for Management levels in ordination.

3. FITTING ENVIRONMENTAL VARIABLES

Vegan provides two functions for fitting environmental variables onto ordination:

- envfit fits vectors of continuous variables and centroids of levels of class variables (defined as factor in R). The direction of the vector shows the direction of the gradient, and the length of the arrow is proportional to the correlation between the variable and the ordination.
- ordisurf (which requires package mgcv) fits smooth surfaces for continuous variables onto ordination using thinplate splines with cross-validatory selection of smoothness.

Function envfit can be called with a formula interface, and it optionally can assess the "significance" of the variables using permutation tests:

```
> ord.fit <- envfit(ord ~ A1 + Management, data = dune.env,</pre>
      perm = 1000)
> ord.fit
***VECTORS
      NMDS1
               NMDS2
                         r2 Pr(>r)
A1 -0.97952 -0.20134 0.3689 0.01798 *
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
P values based on 1000 permutations.
***FACTORS:
Centroids:
               NMDS1
                       NMDS2
{\tt ManagementBF}
              0.4532 -0.0011
ManagementHF
             0.2712 0.1209
ManagementNM -0.3267 -0.5687
```

Goodness of fit:

ManagementSF -0.1259 0.4686

r2 Pr(>r)

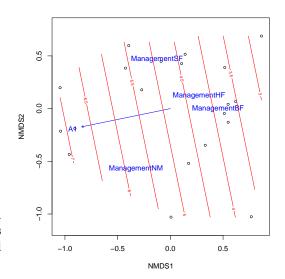


FIGURE 4. Fitted vector and smooth surface for the thickness of A1 horizon (A1, in cm), and centroids of Management levels.

```
Management 0.4206 0.01099 *
---
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' '1
P values based on 1000 permutations.
The result can be drawn directly or added to an ordination diagram (Fig. 4):
> plot(ord, dis = "site")
> plot(ord.fit)
```

Function ordisurf directly adds a fitted surface onto ordination, but it returns the result of the fitted thinplate spline gam (Fig. 4):

```
> ordisurf(ord, A1, add = TRUE)
Family: gaussian
Link function: identity
```

Formula:

 $y \sim s(x1, x2, k = knots)$ <environment: 0x95093d0>

Estimated degrees of freedom:

2 total = 3

GCV score: 3.940943

4. Constrained ordination

Vegan has three methods of constrained ordination: constrained or "canonical" correspondence analysis (function cca), redundancy analysis (function rda) and constrained analysis of proximities (function capscale). All these functions also can have a conditioning term that is "partialled out". I only demonstrate cca, but all functions accept similar commands and can be used in the same way.

The preferred way is to use formula interface, where the left hand side gives the community data frame and the right hand side lists the constraining variables:

```
> ord <- cca(dune ~ A1 + Management, data = dune.env)
> ord
```

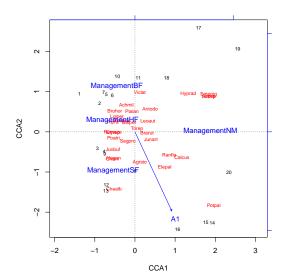


FIGURE 5. Default plot from constrained correspondence analysis.

Call: cca(formula = dune ~ A1 + Management, data = dune.env)

Inertia Proportion Rank

Total 2.1153 1.0000 Constrained 0.7798 0.3686 4 Unconstrained 1.3355 0.6314 15

Inertia is mean squared contingency coefficient

Eigenvalues for constrained axes:

CCA1 CCA2 CCA3 CCA4
0.31875 0.23718 0.13217 0.09168

Eigenvalues for unconstrained axes:

CA1 CA2 CA3 CA4 CA5 CA6 CA7 CA8 0.362024 0.202884 0.152661 0.134549 0.110957 0.079982 0.076698 0.055267 CA9 CA10 CA11 CA12 CA13 CA14 CA15 0.044361 0.041528 0.031699 0.017786 0.011642 0.008736 0.004711

The results can be plotted with (Fig. 5):

> plot(ord)

There are three groups of items: sites, species and centroids (and biplot arrows) of environmental variables. All these can be added individually to an empty plot, and all previously explained tricks of controlling graphics still apply.

It is not recommended to perform constrained ordination with all environmental variables you happen to have: adding the number of constraints means slacker constraint, and you finally end up with solution similar to unconstrained ordination. In that case it is better to use unconstrained ordination with environmental fitting. However, if you really want to do so, it is possible with the following shortcut in formula:

```
> cca(dune ~ ., data = dune.env)
```

Call: cca(formula = dune ~ A1 + Moisture + Management + Use +
Manure, data = dune.env)

Inertia Proportion Rank

Total 2.1153 1.0000

```
Constrained 1.5032 0.7106 12
Unconstrained 0.6121 0.2894 7
```

Inertia is mean squared contingency coefficient

Some constraints were aliased because they were collinear (redundant)

Eigenvalues for constrained axes:

```
CCA1 CCA2 CCA3 CCA4 CCA5 CCA6 CCA7 CCA8 CCA9
0.46713 0.34102 0.17606 0.15317 0.09528 0.07027 0.05887 0.04993 0.03183
CCA10 CCA11 CCA12
0.02596 0.02282 0.01082
```

Eigenvalues for unconstrained axes:

```
CA1 CA2 CA3 CA4 CA5 CA6 CA7 0.27237 0.10876 0.08975 0.06305 0.03489 0.02529 0.01798
```

4.1. Significance tests. Vegan provides permutation tests for the significance of constraints. The test mimics standard analysis of variance function (anova), and the default test analyses all constraints simultaneously:

```
> anova(ord)
```

Permutation test for cca under reduced model

```
Model: cca(formula = dune ~ A1 + Management, data = dune.env)

Df Chisq F N.Perm Pr(>F)

Model 4 0.7798 2.1896 199 0.005 **

Residual 15 1.3355
---

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

The function actually used was <code>anova.cca</code>, but you do not need to give its name in full, because R automatically chooses the correct <code>anova</code> variant for the result of constrained ordination.

The anova.cca function tries to be clever and lazy: it automatically stops if the observed permutation significance probably differs from the targeted critical value (0.05 as default), but it will continue long in uncertain cases. You must set step and perm.max to same values to override this behaviour.

It is also possible to analyse terms separately:

Residual 15 1.3355

```
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
```

In this case, the function is unable to automatically select the number of iterations. This test is sequential: the terms are analysed in the order they happen to be in the model. You can also analyse significances of marginal effects ("Type III effects"):

```
> anova(ord, by = "mar")
```

```
Permutation test for \operatorname{cca} under reduced model Marginal effects of terms
```

```
Model: cca(formula = dune ~ A1 + Management, data = dune.env)
           Df Chisq
                          F N.Perm Pr(>F)
            1 0.1759 1.9761
                               399 0.02 *
A 1
Management 3 0.5550 2.0780
                               199
                                     0.01 **
Residual
           15 1.3355
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
  Moreover, it is possible to analyse significance of each axis:
> anova(ord, by = "axis", perm = 500)
Model: cca(formula = dune ~ A1 + Management, data = dune.env)
                       F N.Perm Pr(>F)
         Df Chisq
                             199 0.005 **
CCA1
          1 0.3187 3.5801
CCA2
          1 0.2372 2.6640
                             199 0.005 **
CCA3
          1 0.1322 1.4845
                             199 0.135
CCA4
          1 0.0917 1.0297
                              99 0.420
Residual 15 1.3355
```

Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' ' 1

Now the automatic selection works, but typically some of your axes will be very close to the critical value, and it may be useful to set a lower perm.max than the default 10000 (typically you use higher limits than in these examples: we used lower limits to save time when this document is automatically generated with this package).

4.2. Conditioned or partial ordination. All constrained ordination methods can have terms that are partialled out from the analysis before constraints:

```
> ord <- cca(dune ~ A1 + Management + Condition(Moisture),
+    data = dune.env)
> ord
Call: cca(formula = dune ~ A1 + Management +
Condition(Moisture), data = dune.env)
```

| Inertia Proportion Rank | Total | 2.1153 | 1.0000 | | Conditional | 0.6283 | 0.2970 | 3 | Constrained | 0.5109 | 0.2415 | 4 | Unconstrained | 0.9761 | 0.4615 | 12

Inertia is mean squared contingency coefficient

```
Eigenvalues for unconstrained axes:
```

```
CA1 CA2 CA3 CA4 CA5 CA6 CA7 CA8
0.306366 0.131911 0.115157 0.109469 0.077242 0.075754 0.048714 0.037582
CA9 CA10 CA11 CA12
0.031058 0.021024 0.012542 0.009277
```

```
This partials out the effect of Moisture before analysing the effects of A1 and
Management. This also influences the significances of the terms:
> anova(ord, by = "term", perm = 500)
Permutation test for cca under reduced model
Terms added sequentially (first to last)
Model: cca(formula = dune ~ A1 + Management + Condition(Moisture), data = dune.env)
           Df Chisq
                         F N.Perm Pr(>F)
            1 0.1154 1.4190
                                    0.16
                                 99
Management 3 0.3954 1.6205
                                 99
                                      0.01 **
Residual
           12 0.9761
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' ' 1
If we had a designed experiment, we may wish to restrict the permutations so that
the observations only are permuted within levels of strata:
> anova(ord, by = "term", perm = 500, strata = Moisture)
Permutation test for cca under reduced model
Terms added sequentially (first to last)
Permutations stratified within 'Moisture'
Model: cca(formula = dune ~ A1 + Management + Condition(Moisture), data = dune.env)
           Df Chisq
                         F N.Perm Pr(>F)
            1 0.1154 1.4190
                                99 0.24
Management 3 0.3954 1.6205
                                 99
                                      0.01 **
Residual 12 0.9761
```

Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1