Vegan: an introduction to ordination

Jari Oksanen

processed with vegan 2.2-0 in R Under development (unstable) (2014-11-16 r66991) on November 17, 2014

Abstract

The document describes typical, simple work pathways of vegetation ordination. Unconstrained ordination uses as examples detrended correspondence analysis and non-metric multidimensional scaling, and shows how to interpret their results by fitting environmental vectors and factors or smooth environmental surfaces to the graph. The basic plotting command, and more advanced plotting commands for congested plots are also discussed, as well as adding items such as ellipses, convex hulls, and other items for classes. The constrained ordination uses constrained (canonical) correspondence analysis as an example. It is first shown how a model is defined, then the document discusses model building and signficance tests of the whole analysis, single constraints and axes.

Contents

1	Ordination	2
	1.1 Detrended correspondence analysis	2
	1.1 Detrended correspondence analysis	2
2	Ordination graphics	3
	2.1 Cluttered plots	4
	2.1 Cluttered plots	5
3	Fitting environmental variables	6
4	Constrained ordination	7
	4.1 Significance tests	9
	4.2 Conditioned or partial ordination	

Vegan is a package for community ecologists. This documents explains how the commonly used ordination methods can be performed 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 nonmetric 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
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 0.14267
Decorana values 0.5360 0.2869 0.08136 0.04814
                3.7004 3.1166 1.30055 1.47888
Axis lengths
```

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 vegan function monoMDS (or alternatively using 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)
Run 0 stress 0.1192678
Run 1 stress 0.1886532
Run 2 stress 0.1183186
... New best solution</pre>
```

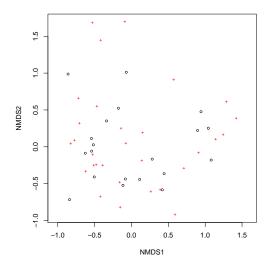


Figure 1: Default ordination plot.

```
... procrustes: rmse 0.02026887 max resid 0.06495011
Run 3 stress 0.1192678
Run 4 stress 0.1183186
... procrustes: rmse 6.471967e-05 max resid 0.000210315
*** Solution reached
> ord
Call:
metaMDS(comm = dune)
{\tt global} \ {\tt Multidimensional} \ {\tt Scaling} \ {\tt using} \ {\tt monoMDS}
Data:
           dune
Distance: bray
Dimensions: 2
             0.1183186
Stress:
Stress type 1, weak ties
Two convergent solutions found after 4 tries
Scaling: centring, PC rotation, halfchange scaling
Species: expanded scores based on 'dune'
```

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

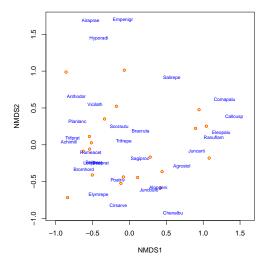


Figure 2: A more colourful ordination plot where sites are points, and species are text.

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:

- 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 add labell only some points with identify command.

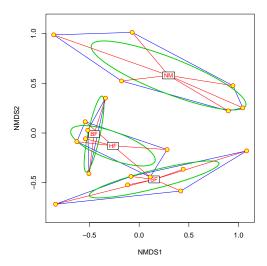


Figure 3: Convex hull, standard error ellipse and a spider web diagram for Management levels in ordination.

- 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):

```
> data(dune.env)
> attach(dune.env)
> plot(ord, disp="sites", type="n")
> ordihull(ord, Management, col="blue")
> ordiellipse(ord, Management, col=3,lwd=2)
> ordispider(ord, Management, col="red", label = TRUE)
> points(ord, disp="sites", pch=21, col="red", bg="yellow", cex=1.3)
```

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.

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 arrow shows the direction of the (increasing) 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, perm=999)</pre>
> ord.fit
***VECTORS
     NMDS1
           NMDS2
                     r2 Pr(>r)
A1 0.96473 0.26325 0.3649 0.017 *
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' ' 1
Permutation: free
Number of permutations: 999
***FACTORS:
Centroids:
              NMDS1 NMDS2
ManagementBF -0.4534 -0.0103
ManagementHF -0.2635 -0.1282
ManagementNM 0.2957 0.5790
ManagementSF 0.1506 -0.4670
Goodness of fit:
              r2 Pr(>r)
Management 0.4134 0.009 **
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Permutation: free
Number of permutations: 999
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):

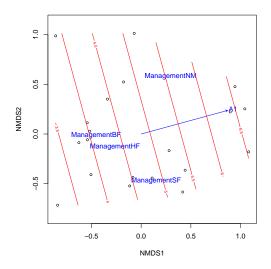


Figure 4: Fitted vector and smooth surface for the thickness of A1 horizon (A1, in cm), and centroids of Management levels.

```
> ordisurf(ord, A1, add=TRUE)
```

Family: gaussian Link function: identity

Formula:

 $y \sim s(x1, x2, k = 10, bs = "tp", fx = FALSE)$

<environment: 0x6e6fa00>

Estimated degrees of freedom:

1.59 total = 2.59

REML score: 41.58727

4 Constrained ordination

Vegan has three methods of constrained ordination: constrained or "canonical" correspondence analysis (function cca), redundancy analysis (function rda) and distance-based redundancy analysis (function capscale). All these functions 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
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

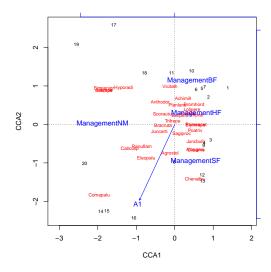


Figure 5: Default plot from constrained correspondence analysis.

Inertia is mean squared contingency coefficient

```
Eigenvalues for constrained axes: CCA1 CCA2 CCA3 CCA4 0.3187 0.2372 0.1322 0.0917
```

```
Eigenvalues for unconstrained axes:
```

```
CA1 CA2 CA3 CA4 CA5 CA6 CA7 CA8 CA9 CA10 0.3620 0.2029 0.1527 0.1345 0.1110 0.0800 0.0767 0.0553 0.0444 0.0415 CA11 CA12 CA13 CA14 CA15 0.0317 0.0178 0.0116 0.0087 0.0047
```

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
```

 ${\tt Inertia\ is\ mean\ squared\ contingency\ coefficient}$

Some constraints were aliased because they were collinear (redundant)

```
Eigenvalues for constrained axes:
         CCA2
               CCA3 CCA4
                              CCA5
                                      CCA6
                                             CCA7
                                                     CCA8
                                                            CCA9 CCA10
0.4671 0.3410 0.1761 0.1532 0.0953 0.0703 0.0589 0.0499 0.0318 0.0260
CCA11 CCA12
0.0228 0.0108
Eigenvalues for unconstrained axes:
            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:

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

It is also possible to analyse terms separately:

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", permutations=199)
```

```
Permutation test for cca under reduced model
Marginal effects of terms
Permutation: free
Number of permutations: 199
Model: cca(formula = dune ~ A1 + Management, data = dune.env)
           Df ChiSquare
                             F Pr(>F)
Α1
                0.17594 1.9761
                                 0.06 .
                0.55502 2.0780
                                 0.01 **
Management 3
Residual
         15
                1.33549
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", permutations=499)
Permutation test for cca under reduced model
Marginal tests for axes
Permutation: free
Number of permutations: 499
Model: cca(formula = dune ~ A1 + Management, data = dune.env)
         Df ChiSquare
                           F Pr(>F)
CCA1
              0.31875 3.5801 0.002 **
          1
CCA2
          1
              0.23718 2.6640 0.004 **
CCA3
          1
              0.13217 1.4845
                             0.102
CCA4
          1
              0.09168 1.0297 0.390
Residual 15
              1.33549
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
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)</pre>
> 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 constrained axes:
           CCA2
                   CCA3
                           CCA4
   CCA1
0.24932 0.12090 0.08160 0.05904
Eigenvalues for unconstrained axes:
    CA1
            CA2
                    CA3
                            CA4
                                    CA5
                                            CA6
                                                    CA7
                                                            CA8
                                                                     CA9
```

```
0.30637 0.13191 0.11516 0.10947 0.07724 0.07575 0.04871 0.03758 0.03106
  CA10 CA11
                 CA12
0.02102 0.01254 0.00928
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", permutations=499)
Permutation test for cca under reduced model
Terms added sequentially (first to last)
Permutation: free
Number of permutations: 499
Model: cca(formula = dune ~ A1 + Management + Condition(Moisture), data = dune.env)
          Df ChiSquare
                           F Pr(>F)
A1
           1 0.11543 1.4190 0.122
Management 3 0.39543 1.6205 0.012 *
Residual 12 0.97610
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 Moisture. Restricted
permutation is based on the powerful permute package. Function how() can
be used to define permutation schemes. In the following, we set the levels with
plots argument:
> how <- how(nperm=499, plots = Plots(strata=dune.env$Moisture))</pre>
> anova(ord, by="term", permutations = how)
Permutation test for cca under reduced model
Terms added sequentially (first to last)
Plots: dune.env$Moisture, plot permutation: none
Permutation: free
Number of permutations: 499
Model: cca(formula = dune ~ A1 + Management + Condition(Moisture), data = dune.env)
          Df ChiSquare
                           F Pr(>F)
           1 0.11543 1.4190 0.242
              0.39543 1.6205 0.002 **
Management 3
Residual 12 0.97610
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
```