Vegan: an introduction to ordination

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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.

Keywords: ordination, correspondence analysis, non-metric multidimensional scaling, CCA, RDA, NMDS, fitted environmental vector, fitted environmental surface, permutation tests.

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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 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:

```
R> library(vegan)
R> data(dune)
R> ord <- decorana(dune)</pre>
```

This saves ordination results in ord:

```
R> 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 0.14266
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 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):

```
R> ord <- metaMDS(dune)</pre>
Run 0 stress 0.1192691
Run 1 stress 0.1192693
... procrustes: rmse 0.0007240573 max resid 0.001887997
*** Solution reached
R> ord
Call:
metaMDS(comm = dune)
global Multidimensional Scaling using monoMDS
Data:
          dune
Distance: bray
Dimensions: 2
Stress:
         0.1192691
Stress type 1, weak ties
Two convergent solutions found after 1 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):

```
R> 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):

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

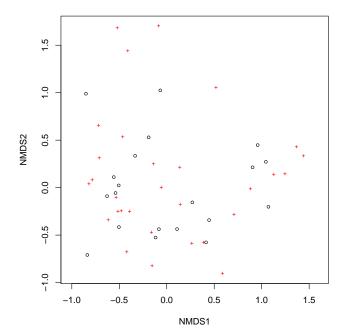


Figure 1: Default ordination plot.

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.
- 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.

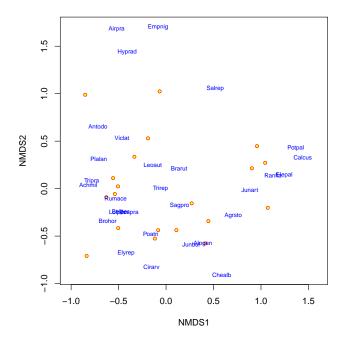


Figure 2: A more colourful ordination plot where sites are points, and species are text.

• 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):

```
R> data(dune.env)
R> attach(dune.env)

R> plot(ord, disp = "sites", type = "n")
R> ordihull(ord, Management, col = "blue")
R> ordiellipse(ord, Management, col = 3, lwd = 2)
R> ordispider(ord, Management, col = "red", label = TRUE)
R> 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:

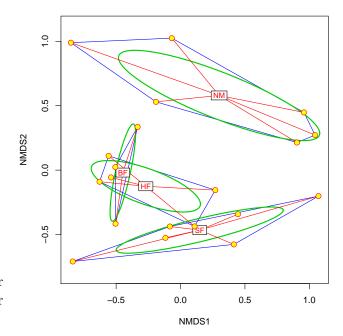


Figure 3: Convex hull, standard error ellipse and a spider web diagram for Management levels in ordination.

- 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:

```
R> ord.fit <- envfit(ord ~ A1 + Management, data = dune.env,</pre>
       perm = 1000)
R> ord.fit
***VECTORS
                     r2 Pr(>r)
     NMDS1
             NMDS2
A1 0.99055 0.13712 0.38 0.02098 *
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' ' 1
P values based on 1000 permutations.
***FACTORS:
Centroids:
               NMDS1
                       NMDS2
ManagementBF -0.4478 -0.0190
ManagementHF -0.2695 -0.1255
ManagementNM 0.2995 0.5797
```

```
ManagementSF 0.1490 -0.4656
Goodness of fit:
                     Pr(>r)
                r2
Management 0.4142 0.004995 **
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):
R> plot(ord, dis = "site")
R> 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):
R> ordisurf(ord, A1, add = TRUE)
Family: gaussian
Link function: identity
Formula:
y \sim s(x1, x2, k = knots)
<environment: 0x1026cf228>
Estimated degrees of freedom:
2 \text{ total} = 3
```

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:

GCV score: 3.871584

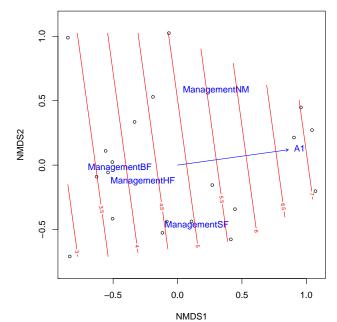


Figure 4: Fitted vector and smooth surface for the thickness of A1 horizon (A1, in cm), and centroids of Management levels.

Inertia is mean squared contingency coefficient

```
Eigenvalues for unconstrained axes:
```

```
CA6
                                                                       CA8
     CA1
              CA2
                        CA3
                                 CA4
                                           CA5
                                                              CA7
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):

```
R> 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:

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

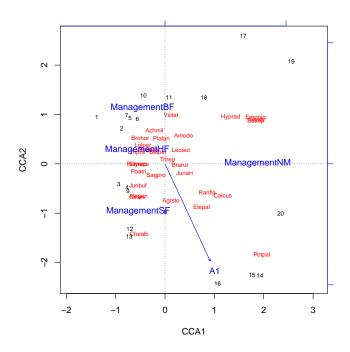


Figure 5: Default plot from constrained correspondence analysis.

```
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:

R> anova(ord)

Permutation test for cca under reduced model

```
Residual 15 1.3355
---
Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
```

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.

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:

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"):

```
R> anova(ord, by = "mar")
Permutation test for cca under reduced model
Marginal effects of terms
Model: cca(formula = dune ~ A1 + Management, data = dune.env)
                        F N.Perm Pr(>F)
          Df Chisq
            1 0.1759 1.9761
                            1099 0.03364 *
Management 3 0.5550 2.0780
                              199 0.00500 **
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:
R> anova(ord, by = "axis", perm = 500)
Model: cca(formula = dune ~ A1 + Management, data = dune.env)
        Df Chisq
                      F N.Perm Pr(>F)
          1 0.3187 3.5801
                            199 0.010 **
CCA1
CCA2
                            199 0.015 *
          1 0.2372 2.6640
```

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:

```
R> ord <- cca(dune ~ A1 + Management + Condition(Moisture),</pre>
       data = dune.env)
R> 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
               0.5109
                           0.2415
                                     4
Constrained
                                    12
Unconstrained 0.9761
                           0.4615
Inertia is mean squared contingency coefficient
Eigenvalues for constrained axes:
   CCA1
           CCA2
                   CCA3
                            CCA4
0.24932 0.12090 0.08160 0.05904
Eigenvalues for unconstrained axes:
     CA1
              CA2
                       CA3
                                 CA4
                                          CA5
                                                    CA6
                                                             CA7
                                                                       CAS
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:

Residual 12 0.9761

```
Signif. codes: 0 '***' 0.001 '**' 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:

R> 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)

A1 1 0.1154 1.4190 99 0.31

Management 3 0.3954 1.6205 99 0.02 *

Residual 12 0.9761
---
```

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

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