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 significance tests of the whole analysis, single constraints and axes.

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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. 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
Call:
decorana(veg = dune)
Detrended correspondence analysis with 26 segments.
Rescaling of axes with 4 iterations.
Total inertia (scaled Chi-square): 2.1153
                              DCA2
                                       DCA3
                       DCA1
                     0.5117 0.3036 0.12125 0.14267
Eigenvalues
Additive Eigenvalues 0.5117 0.2985 0.12242 0.12984
```

Additive Eigenvalues 0.5117 0.2985 0.12242 0.12984

Decorana values 0.5360 0.2869 0.08136 0.04814

Axis lengths 3.7004 3.1166 1.30055 1.47888

The display of results is very brief: only eigenvalues and used options are listed.

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, trace = FALSE)
> ord
Call:
metaMDS(comm = dune, trace = FALSE)
global Multidimensional Scaling using monoMDS
Data: dune
```

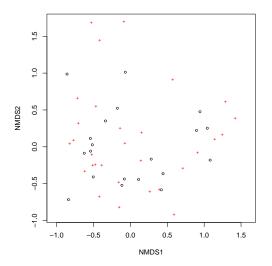


Figure 1: Default ordination plot.

Distance: bray

Dimensions: 2

Stress: 0.1183186 Stress type 1, weak ties

Best solution was repeated 10 times in 20 tries The best solution was from try 4 (random start) 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 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 = "species", cex=0.7, col="blue")
```

The plot commands can be chained with pipe |>, and the previous can also be expressed as:

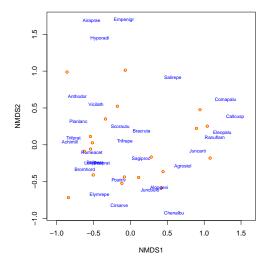


Figure 2: A more colourful ordination plot where sites are points, and species are text.

```
> plot(ord, type = "n") |>
points("sites", cex = 0.8, pch=21, col="red", bg="yellow") |>
text("species", 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**).

Alternative plotting methods are available in two packages:

- **vegan3d** in CRAN provides static 3D plots (ordiplot3d), dynamic 3D plots that can be spinned around or zoomed (ordirg1) and interactive 2D plots that can be edited moving point labels to better position (orditkplot).
- ggvegan in github provides ggplot2 graphics for most vegan objects. The vegan scores functions for ordination objects (and some others) recognize argument tidy which can be used to extract scores for ggplot2 graphics. NB., there are some lattice graphics functions in vegan, but the plan is to phase out these in favour of ggvegan graphics.

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 label only to some points with identify command.

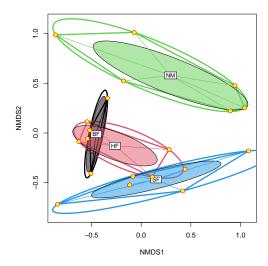


Figure 3: Convex hull, ellipsoid hull, standard error ellipse and a spider web diagram for Management levels in ordination.

- 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 in vegan3d that draws both points and labels for ordination scores, and allows you to drag labels to better positions. You can export the edited graph in several graphical formats, 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 enclosing all points in the group (ellipsoid hulls) or 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=1:4, lwd=3)
> ordiellipse(ord, Management, col=1:4, kind = "ehull", lwd=3)
> ordiellipse(ord, Management, col=1:4, draw="polygon")
> ordispider(ord, Management, col=1:4, 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 0.96474 0.26322 0.3649 0.022 *
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 -0.0102
ManagementHF -0.2636 -0.1282
ManagementNM 0.2958 0.5790
ManagementSF 0.1506 -0.4670
Goodness of fit:
              r2 Pr(>r)
Management 0.4134 0.012 *
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)
```

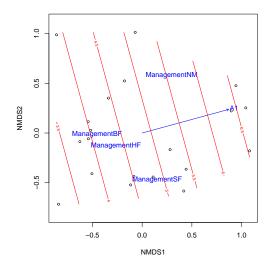


Figure 4: Fitted vector and smooth surface for the thickness of A1 horizon (A1, in cm), and centroids of Management levels.

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 ~ s(x1, x2, k = 10, bs = "tp", fx = FALSE)

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 dbrda). 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)
-- Model Summary --
```

Inertia Proportion Rank

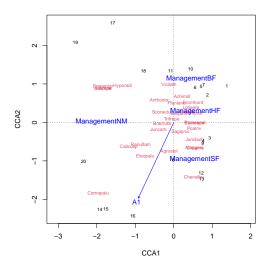


Figure 5: Default plot from constrained correspondence analysis.

```
Total 2.1153 1.0000
Constrained 0.7798 0.3686 4
Unconstrained 1.3355 0.6314 15
```

Inertia is scaled Chi-square

```
-- Eigenvalues --
```

```
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
                                                CA7
                                                       CA8
                                                               CA9
                                        CA6
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)
```

-- Model Summary --

Inertia is scaled Chi-square

-- Note --

Some constraints or conditions were aliased because they were redundant. This can happen if terms are linearly dependent (collinear): 'Manure^4'

-- Eigenvalues --

Eigenvalues for constrained axes:

CCA1 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:

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

Permutation: free

Number of permutations: 999

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

Df ChiSquare F Pr(>F)

Model 4 0.77978 2.1896 0.001 ***

Residual 15 1.33549

Signif. codes: 0 '*** 0.001 '** 0.01 '* 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.

It is also possible to analyse terms separately:

> anova(ord, by="term", permutations=199)

Permutation test for cca under reduced model Terms added sequentially (first to last) Permutation: free

```
Number of permutations: 199
Model: cca(formula = dune ~ A1 + Management, data = dune.env)
           Df ChiSquare
                           F Pr(>F)
                0.22476 2.5245 0.015 *
Management 3
               0.55502 2.0780 0.005 **
Residual
         15
               1.33549
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
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)
               0.17594 1.9761 0.015 *
Management 3
               0.55502 2.0780 0.010 **
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
Forward 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 0.014 *
         1
CCA2
             0.23718 2.6640 0.142
         1
CCA3
             0.13217 1.4845 0.848
         1
CCA4
             0.09168 1.0297 1.000
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)
> ord
```

```
Call: cca(formula = dune ~ A1 + Management + Condition(Moisture),
data = dune.env)
-- Model Summary --
              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 scaled Chi-square
-- Eigenvalues --
Eigenvalues for constrained axes:
           CCA2
                   CCA3
                           CCA4
0.24932 0.12090 0.08160 0.05904
Eigenvalues for unconstrained axes:
                                     CA5
                                             CA6
                                                     CA7
                                                              CA8
                                                                      CA9
    CA1
            CA2
                    CA3
                            CA4
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)
                0.11543 1.4190 1.000
A 1
            1
Management 3
                0.39543 1.6205 0.002 **
                0.97610
Residual
          12
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)

A1 1 0.11543 1.4190 1.000

Management 3 0.39543 1.6205 0.002 **

Residual 12 0.97610

---

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