Basic Ordination

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Introduction

Introduction

- Ordination comes from the German word *ordnung*, meaning to put things in order
- This is exactly what we we do in ordination — we arrange our samples along gradients by fitting lines and planes through the data that describe the main patterns in those data
- Linear and unimodal methods
- Principle Components Analysis (PCA) is a linear method — most useful for environmental data or sometimes with species data and short gradients
- Correspondence Analysis (CA) is a unimodal method — most useful for species data, especially where non-linear responses are observed

Principal Components Analysis

Ordination

- Regression gives us a basis from which to work
- Instead of doing many regressions, do one with all the species data once
- Only now we don't have any explanatory variables, we wish to uncover these underlying gradients
- PCA fits a line through our cloud of data in such a way that it maximises the variance in the data captured by that line (i.e.~minimises the distance between the fitted line and the observations)
- Then we fit a second line to form a plane, and so on, until we have one PCA line or axis for each of our species
- Each of these subsequent axes is uncorrelated with previous axes — they are orthogonal — so the variance each axis explains is uncorrelated

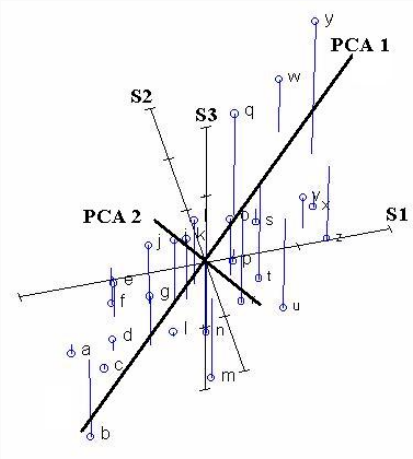
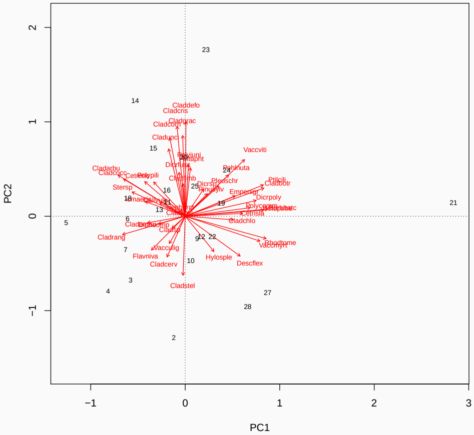


Figure 1:

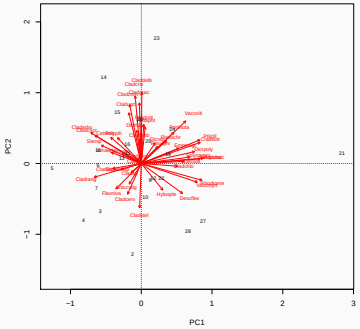
Vegetation in lichen pastures — PCA

Data are cover values of 44 understorey species recorded at 24 locations in lichen pastures within dry *Pinus sylvestris* forests



Vegetation in lichen pastures — PCA biplots

- Have two sets of scores
    - Species scores
    - Site scores \end{enumerate}
- Sample (species) points plotted close together have similar species compositions (occur together)
- In PCA, species scores often drawn as arrows — point in direction of increasing abundance
- Species arrows with small angles to an axis are highly correlated with that axis



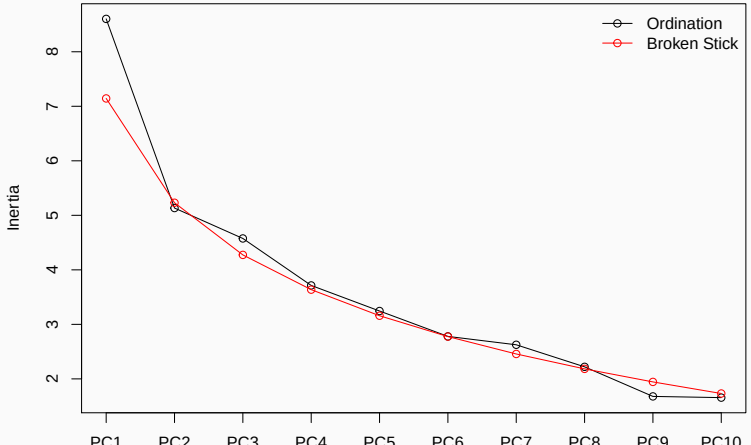
Eigenvalues

Eigenvalues λ are the amount of variance (inertia) explained by each axis

```
head(eigenvals(pca), 6L)
```

```
      PC1       PC2       PC3       PC4       PC5       PC6 
8.602826 5.133623 4.575623 3.713926 3.244925 2.779195 
```

```
screeplot(pca, bstick = TRUE, type = "l", main = NULL)
```

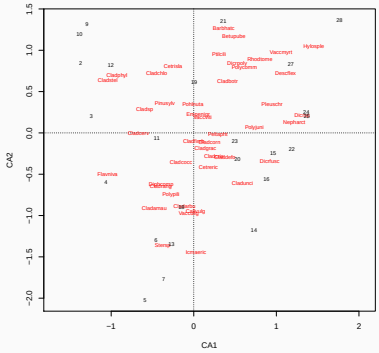


Correspondence Analysis

Correspondence Analysis

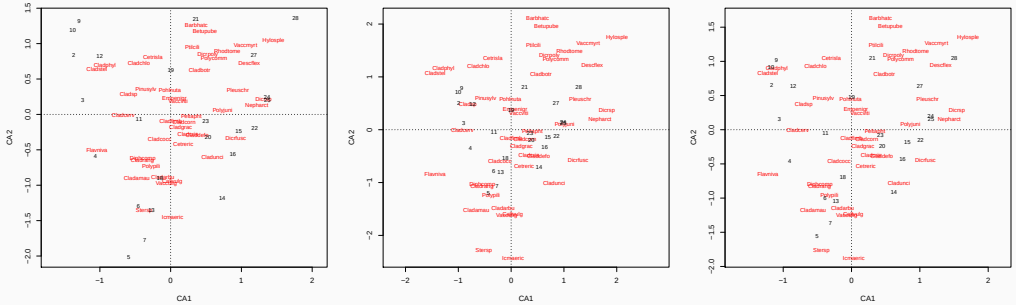
Vegetation in lichen pastures — CA biplots

- Have two sets of scores
    1. Species scores
    2. Site scores
- Sample (species) points plotted close together have similar species compositions (occur together)
- In CA, species scores drawn as points — this is the fitted optima along the gradients
- Abundance of species declines in concentric circles away from the optima



Vegetation in lichen pastures — CA biplots

- Species scores plotted as weighted averages of site scores, or
- Site scores plotted as weighted averages of species scores, or
- A symmetric plot



Vegan usage

Vegan basics

- The majority of vegan functions work with a single vector, or more commonly an entire data frame
- This data frame may contain the species abundances
- Where subsidiary data is used/required, these two are supplied as data frames
- For example; the environmental constraints in a CCA
- It is not a problem if you have all your data in a single file/object; just subset it into two data frames after reading it into R

```
spp <- allMyData[, 1:20] ## columns 1-20 contain the species data
env <- allMyData[, 21:26] ## columns 21-26 contain the environmental data
```

Simple vegan usage

First we start with a simple correspondence analysis (CA) to illustrate the basic features

Here I am using one of the in-built data sets on lichen pastures

For various reasons to fit a CA we use the `cca()` function

Store the fitted CA in `ca1` and print it to view the results

```
ca1 <- cca(varespec)
ca1
```

```
Call: cca(X = varespec)

              Inertia Rank
Total           2.083
Unconstrained   2.083   23
Inertia is mean squared contingency coefficient

Eigenvalues for unconstrained axes:
   CA1    CA2    CA3    CA4    CA5    CA6    CA7    CA8
0.5249 0.3568 0.2344 0.1955 0.1776 0.1216 0.1155 0.0889
(Showed only 8 of all 23 unconstrained eigenvalues)
```

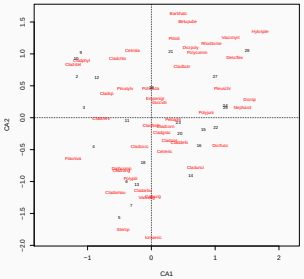
`scores()` & `scaling` in `cca()`, `rda()`

- When we draw the results of many ordinations we display 2 or more sets of data
- Can't display all of these and maintain relationships between the scores
- Solution; scale one set of scores relative to the other
- Controlled via the `scaling` argument
  - `scaling = 1` — Focus on species, scale site scores by λ_i
  - `scaling = 2` — Focus on sites, scale species scores by λ_i
  - `scaling = 3` — Symmetric scaling, scale both scores by $\sqrt{\lambda_i}$
  - `scaling = -1` — As above, but
  - `scaling = -2` — For `cca()` multiply results by $\sqrt{(1/(1-\lambda_i))}$
  - `scaling = -3` — this is Hill's scaling
  - `scaling < 0` — For `rda()` divide species scores by species' σ
  - `scaling = 0` — raw scores

Basic ordination plots

- Basic plotting can be done using the `plot()` method
- `choices = 1:2` — select which axes to plot
- `scaling = 3` — scaling to use
- `display = c("sites","species")` — which scores (default is both)
- `type = "text"` — display scores using labels or points (`"points"`)
- Other graphics arguments can be supplied but the apply for all scores

```
plot(ca1, scaling = "symmetric")
```



Non-Metric Multidimensional Scaling

Non-Metric Multidimensional Scaling

- Aim is to find a low-dimensional mapping of dissimilarities
- Similar idea to PCoA, but does not use the actual dissimilarities
- NMDS attempts to find a low-dimensional mapping that preserves as best as possible the rank order of the original dissimilarities (d_{ij})
- Solution with minimal `stress` is sought; a measure of how well the NMDS mapping fits the d_{ij}
- Stress is sum of squared residuals of monotonic regression between distances in NMDS space (d^*_{ij}) & d_{ij}
- Non-linear regression can cope with non-linear responses in species data
- Iterative solution; convergence is not guaranteed
- Must solve separately different dimensionality solutions

Non-Metric Multidimensional Scaling

- Use an appropriate dissimilarity metric that gives good gradient separation `rankindex()`
  - Bray-Curtis
  - Jaccard
  - Kulczynski
- Wisconsin transformation useful; Standardize species to equal maxima, then sites to equal totals `wisconsin()`
- Iterative solution; use many random starts and look at the fits with lowest stress
- Only conclude solution reached if lowest stress solutions are similar (Procrsutes rotation)
- Fit NMDS for 1, 2, 3, ...dimensions; stop after a sudden drop in stress observed in a screeplot
- NMDS solutions can be rotated at will; common to rotate to principal components
- Also scale axes in half-change units; samples separated by a distance of 1 correspond, on average, to a 50% turnover in composition

NMDS in vegan

Vegan implements all these ideas via the `metaMDS()` wrapper

```
data(dune)
set.seed(10)
(sol <- metaMDS(dune, trace = FALSE))
```

```
Call:
metaMDS(comm = dune, trace = FALSE)

global Multidimensional Scaling using monoMDS

Data:     dune
Distance: bray

Dimensions: 2
Stress:     0.1183186
Stress type 1, weak ties
Two convergent solutions found after 20 tries
Scaling: centring, PC rotation, halfchange scaling
Species: expanded scores based on 'dune'
```

NMDS in vegan

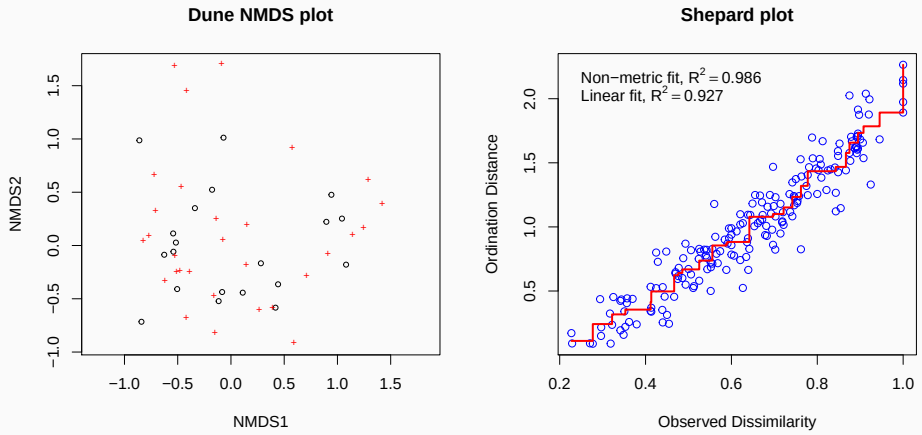
If no convergent solutions, continue iterations from previous best solution

```
(sol <- metaMDS(dune, previous.best = sol, trace = FALSE))
```

```
Call:
metaMDS(comm = dune, trace = FALSE, previous.best = sol)

global Multidimensional Scaling using monoMDS

Data:     dune
Distance: bray

Dimensions: 2
Stress:     0.1183186
Stress type 1, weak ties
Two convergent solutions found after 40 tries
Scaling: centring, PC rotation, halfchange scaling
Species: expanded scores based on 'dune'
```

NMDS in vegan

```
layout(matrix(1:2, ncol = 2))
plot(sol, main = "Dune NMDS plot")
stressplot(sol, main = "Shepard plot")
layout(1)
```



Links

I have several **vegan**-related posts on my blog. For a list of posts see http://www.fromthebottomoftheheap.net/blog/

Re-use