An Introduction to R for the Geosciences: Ordination

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Outline

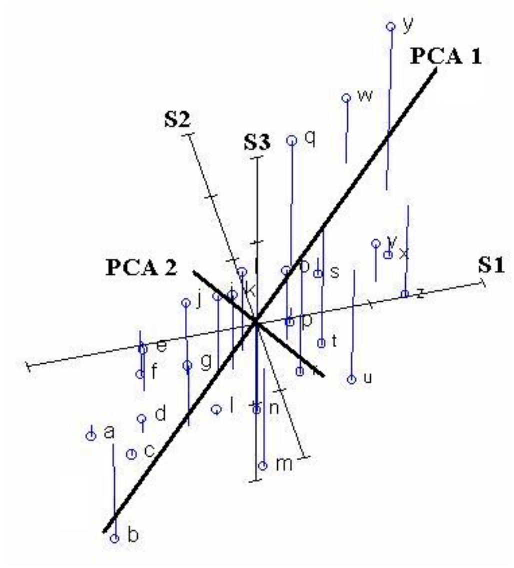
Ordination

- 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

Ordination

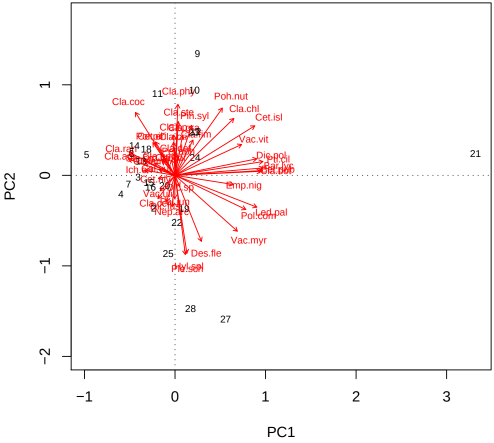
- Regression gives us a basis from which to work
- Instead of doing many regressions, do one with all the species data once
- Only now we don't have any explanatory variables, we wish to uncover these underlying gradients
- PCA fits a line through our cloud of data in such a way that it maximises the 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

Ordination



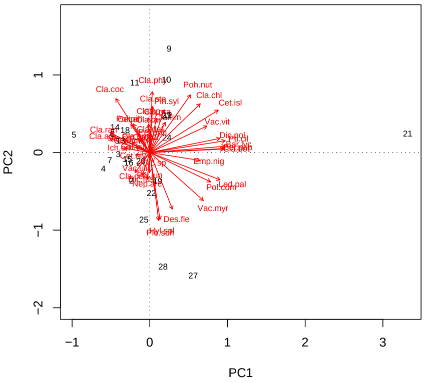
Vegetation in lichen pastures — PCA

- 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

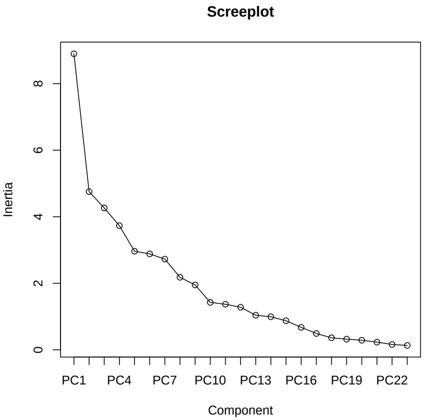
- Have two sets of scores
  1. Species scores
  2. Site scores
- Sample (species) points plotted close together have similar species compositions (occur together)
- In PCA, species scores often drawn as arrows — point in direction of increasing abundance
- Species arrows with small angles to an axis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



Eigenvalues

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

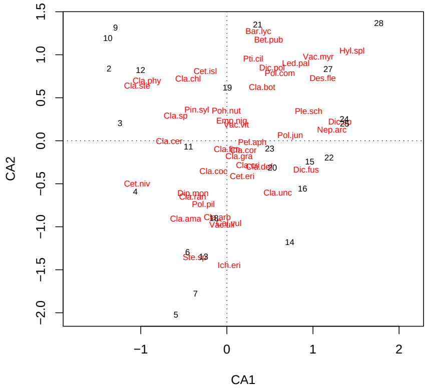
```
             PC1    PC2    PC3    PC4
lambda    8.8984 4.7556 4.2643 3.732
accounted 0.2022 0.3103 0.4072 0.492
```



Correspondence Analysis

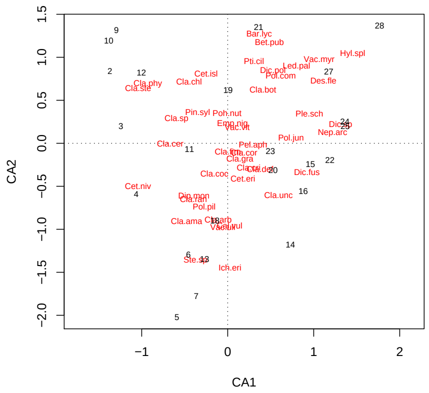
Vegetation in lichen pastures — CA biplots

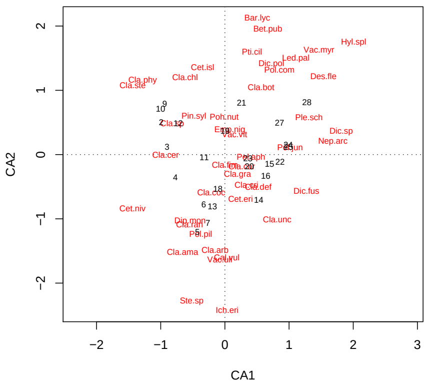
- Have two sets of scores
  1. Species scores
  2. Site scores
- Sample (species) points plotted close together have similar species compositions (occur together)
- In CA, species scores drawn as points — this is the fitted optima along the gradients
- Abundance of species declines in concentric circles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





Outline

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
```

Loading vegan for use

- As with any package, vegan needs to be loaded into the R session before it can be used
- When vegan loads it displays a simple message showing the version number
- Note also that vegan depends upon the permute package

```
> library("vegan")
```

Simple vegan usage; basic ordination

- 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

```
> data(varespec)
> 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)
```

Simple vegan usage; basic ordination

```
> class(ca1)

[1] "cca"

> str(ca1, max = 1) ## top level components

List of 10
 $ call       : language cca(X = varespec)
 $ grand.total: num 2418
 $ rowsum     : Named num [1:24] 0.0369 0.0372 0.039 0.052 0.0374 ...
  ..- attr(*, "names")= chr [1:24] "18" "15" "24" "27" ...
 $ colsum     : Named num [1:44] 0.01864 0.06287 0.00347 0.02097 0.11376 ...
  ..- attr(*, "names")= chr [1:44] "Cal.vul" "Emp.nig" "Led.pal" "Vac.myr" ...
 $ tot.chi    : num 2.08
 $ pCCA       : NULL
 $ CCA        : NULL
 $ CA         :List of 8
 $ method     : chr "cca"
 $ inertia    : chr "mean squared contingency coefficient"
 - attr(*, "class")= chr "cca"
```

The CCA object `?cca.object`

- Objects of class `"cca"` are complex with many components
- Entire class described in `?cca.object`
- Depending on what analysis performed some components may be `NULL`
- Used for (C)CA, PCA, RDA, and CAP (`capscale()`)
- `ca1` has:
  - `$call` how the function was called
  - `$grand.total` in (C)CA sum of `rowsum`
  - `$rowsum` the row sums
  - `$colsum` the column sums
  - `$tot.chi` total inertia, sum of Eigenvalues
  - `$pCCA` Conditioned (partialled out) components
  - `$CCA` Constrained components
  - `$CA` Unconstrained components
  - `$method` Ordination method used
  - `$inertia` Description of what inertia is

The CCA object `?cca.object`

- The `$pCCA` `$CCA`, and `$CA` components contain a number of other components
- Most usefully the Eigenvalues are found here plus the species (variables) and site (samples) score
- `ca1$CA` has:
  - `$eig` the Eigenvalues (λ)
  - `$u` (weighted) orthonormal site scores
  - `$v` (weighted) orthonormal species scores
  - `$u.eig` `u` scaled by λ
  - `$v.eig` `v` scaled by λ
  - `$rank` the rank or dimension of component (number of axes)
  - `$tot.chi` sum of λ for this component
  - `$Xbar` the standardised data matrix after previous stages of analysis
- `*.eig` may disappear in a future version of vegan
- There are many other components that may be present in more complex analyses (e.g. CCA)

Extractor functions — eigenvals()

- Thankfully we don't need to remember all those components in general use — extractor functions
- To extract the eigenvalues use eigenvals():

```
> eigenvals(ca1)
```

```
      CA1       CA2       CA3       CA4       CA5       CA6       CA7       CA8 
0.5249320 0.3567980 0.2344375 0.1954632 0.1776197 0.1215603 0.1154922 0.0889385 
      CA9      CA10      CA11      CA12      CA13      CA14      CA15      CA16 
0.0731751 0.0575174 0.0443421 0.0254635 0.0171030 0.0148963 0.0101598 0.0078298 
     CA17      CA18      CA19      CA20      CA21      CA22      CA23 
0.0060323 0.0040079 0.0028650 0.0019275 0.0018074 0.0005864 0.0002434 
```

Extractor functions — scores()

- The scores() function is an important extractor if you want to access any of the results for use elsewhere
- Takes an ordination object as the first argument
- choices: which axes to return scores for, defaults to c(1,2)
- display: character vector of the type(s) of scores to return

```
> str(scores(ca1, choices = 1:4, display = c("species","sites")))

List of 2
 $ species: num [1:44, 1:4] 0.022 0.0544 0.8008 1.0589 0.1064 ...
  ..- attr(*, "dimnames")=List of 2
  .. ..$ : chr [1:44] "Cal.vul" "Emp.nig" "Led.pal" "Vac.myr" ...
  .. ..$ : chr [1:4] "CA1" "CA2" "CA3" "CA4"
 $ sites  : num [1:24, 1:4] -0.149 0.962 1.363 1.176 0.497 ...
  ..- attr(*, "dimnames")=List of 2
  .. ..$ : chr [1:24] "18" "15" "24" "27" ...
  .. ..$ : chr [1:4] "CA1" "CA2" "CA3" "CA4"

> head(scores(ca1, choices = 1:2, display = "sites"))

            CA1         CA2
18 -0.149231732 -0.89909538
15  0.962176641 -0.24176673
24  1.363110128  0.25182197
27  1.175623286  0.83540787
23  0.496714476 -0.09389079
```

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

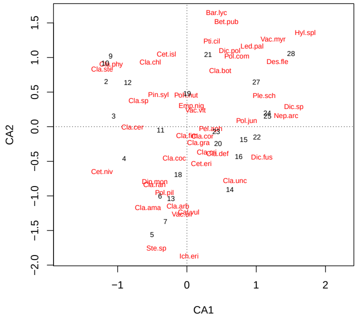
- When we draw the results of many ordinations we display 2 or more sets of data
- Can't display all of these and maintain relationships between the scores
- Solution; scale one set of scores relative to the other
- Controlled via the `scaling` argument
  - `scaling = 1` — Focus on species, scale site 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

```
> scores(ca1, choices = 1:2, display = "species", scaling = 3)
```

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
- See `?plot.cca` for details
- Customisation tricky — better to plot by hand (tomorrow)

```
> plot(ca1, scaling = 3)
```



Outline

Indirect gradient analysis

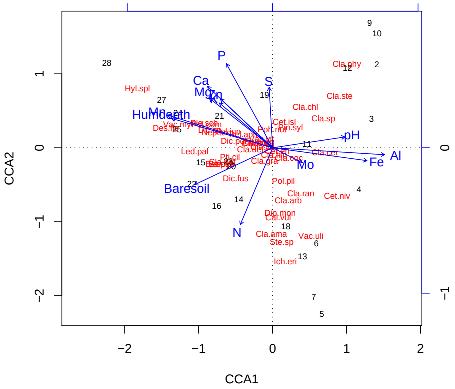
- PCA and CA are indirect gradient analysis methods
- First extract the hypothetical gradients (axes), then relate these gradients to measured environmental data using regression
- But what happens if the gradients extracted are only partly explained by your measured data?
- Or, what if your measured data do not explain the main patterns (axes 1 and 2 say) in the species data, but are important on later axes?
- Direct gradient analysis allows us to do the ordination and regression in one single step
- As before there are linear and unimodal methods:
    - Redundancy Analysis (RDA) is a linear method, the counterpart to PCA
    - Canonical (Constrained) Correspondence Analysis (CCA) is a unimodal method, the counterpart to CA

Direct gradient analysis

- In PCA and CA we fitted lines and curves that fitted the data best — explained most variance
- In RDA and CCA we still fit lines and curves, but we are constrained in how we can fit these axes
- In RDA/CCA we can only fit axes that are linear combinations of our measured environmental data
- By linear combinations, we mean $(2 \times \mathrm{pH}) + (1.5 \times \mathrm{moisture})$
- In other words, we constrain the ordination axes such that the patterns/gradients extracted are restricted to those that we can explain with the measured data

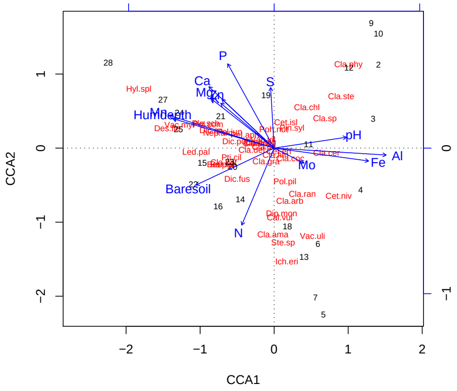
Vegetation in lichen pastures — CCA

- Now we fit a CCA to the lichen pasture data, constrained by the measured environmental data



Vegetation in lichen pastures — CCA triplots

- Triplots show 3 bits of information — compromise
- Species and site scores plotted along side biplot arrows for environmental data
- Sites close together have similar species and environments
- Species close together occur together
- Angles between arrows reflect correlations between env variables
- Length of arrows indicate importance of variable — longer variables more important



Vegetation in lichen pastures — CCA

```
Eigenvalues, and their contribution
             CCA1   CCA2   CCA3   CCA4
lambda     0.4389 0.2918 0.1628 0.1421
accounted  0.2107 0.3507 0.4289 0.4971
```

- Again, Eigenvalues λ are measured of variance explained
- As this is constrained, λ will be lower than in unconstrained methods
- One problem is that as we increase the number of environmental variables as explanatory variable, we actually reduce the constraints on the ordination
- Can only have $\min(\mathrm{n}_{\mathrm{species}}, \mathrm{n}_{\mathrm{samples}}) - 1$ CCA axes but then constraints are 0 and we have the same result as CA
- As CCA/RDA are regression techniques, we should try to reduce the number of explanatory variables down to only those variables that are important for explaining the species composition

Fitting constrained ordinations

- Vegan has two interfaces to specify the model fitted; basic,

```
> data(varechem)
> cca1 <- cca(X = varespec, Y = varechem)
```

- or formula

```
> cca1 <- cca(varespec ~ ., data = varechem)
```

- Formula interface is more powerful and is recommended

```
> cca1

Call: cca(formula = varespec ~ N + P + K + Ca + Mg + S + Al + Fe + Mn +
Zn + Mo + Baresoil + Humdepth + pH, data = varechem)

              Inertia Proportion Rank
Total          2.0832     1.0000
Constrained    1.4415     0.6920   14
Unconstrained  0.6417     0.3080    9
Inertia is mean squared contingency coefficient

Eigenvalues for constrained axes:
  CCA1   CCA2   CCA3   CCA4   CCA5   CCA6   CCA7   CCA8   CCA9  CCA10  CCA11
0.4389 0.2918 0.1628 0.1421 0.1180 0.0890 0.0703 0.0584 0.0311 0.0133 0.0084
 CCA12  CCA13  CCA14
0.0065 0.0062 0.0047

Eigenvalues for unconstrained axes:
    CA1     CA2     CA3     CA4     CA5     CA6     CA7     CA8     CA9
0.19776 0.14193 0.10117 0.07079 0.05330 0.03330 0.01887 0.01510 0.00949
```

Fitting constrained ordinations

- A better approach is to think about the important variables and include only those
- The formula interface allows you to create interaction or quadratic terms easily (though be careful with latter)
- It also handles factor or class constraints automatically unlike the basic interface

```
> vare.cca <- cca(varespec ~ Al + P*(K + Baresoil), data = varechem)
> vare.cca

Call: cca(formula = varespec ~ Al + P * (K + Baresoil), data =
varechem)

              Inertia Proportion Rank
Total           2.083      1.000
Constrained     1.046      0.502    6
Unconstrained   1.038      0.498   17
Inertia is mean squared contingency coefficient

Eigenvalues for constrained axes:
  CCA1   CCA2   CCA3   CCA4   CCA5   CCA6
0.3756 0.2342 0.1407 0.1323 0.1068 0.0561

Eigenvalues for unconstrained axes:
    CA1     CA2     CA3     CA4     CA5     CA6     CA7     CA8
0.27577 0.15411 0.13536 0.11803 0.08887 0.05511 0.04919 0.03781
(Showed only 8 of all 17 unconstrained eigenvalues)
```

Fitting partial constrained ordinations

- The effect of one or more variables can be partialled out by supplying them as object `Z` in the basic interface
- The formula interface can be used too, via a special function `Condition()`

```
> pcca <- cca(varespec ~ Ca + Condition(pH), data = varechem)
> pcca

Call: cca(formula = varespec ~ Ca + Condition(pH), data = varechem)

              Inertia Proportion Rank
Total          2.0832     1.0000
Conditional    0.1458     0.0700    1
Constrained    0.1827     0.0877    1
Unconstrained  1.7547     0.8423   21
Inertia is mean squared contingency coefficient

Eigenvalues for constrained axes:
   CCA1
0.18269

Eigenvalues for unconstrained axes:
   CA1    CA2    CA3    CA4    CA5    CA6    CA7    CA8
0.3834 0.2749 0.2123 0.1760 0.1701 0.1161 0.1089 0.0880
(Showed only 8 of all 21 unconstrained eigenvalues)
```

Model Building

- Automatic approaches to model building should be used cautiously
- The standard `step()` function can be used as vegan provides two helper methods; `deviance()` and `extractAIC()` used by `step()`
- Vegan also provides methods for class `"cca"` for `add1()` and `drop1()`.
- To use, we define an upper and lower model scope, say the full model and the null model
- To step from the lower scope or null model we use

```
> upr <- cca(varespec ~ ., data = varechem)
> lwr <- cca(varespec ~ 1, data = varechem)
> mods <- step(lwr, scope = formula(upr), test = "perm", trace = 0)
```

- `trace = 0` is used her to turn off printing of progress
- `test = "perm"` indicates permutation tests are used (more on these later); the theory for an AIC for ordination is somewhat loose

Model Building

- The object returned by `step()` is a standard `"cca"` object with an extra component `$anova`
- The `$anova` component contains a summary of the steps involved in automatic model building

```
> mods

Call: cca(formula = varespec ~ Al + P + K, data = varechem)

              Inertia Proportion Rank
Total          2.0832     1.0000
Constrained    0.6441     0.3092    3
Unconstrained  1.4391     0.6908   20
Inertia is mean squared contingency coefficient

Eigenvalues for constrained axes:
  CCA1   CCA2   CCA3
0.3616 0.1700 0.1126

Eigenvalues for unconstrained axes:
   CA1    CA2    CA3    CA4    CA5    CA6    CA7    CA8
0.3500 0.2201 0.1851 0.1551 0.1351 0.1003 0.0773 0.0537
(Showed only 8 of all 20 unconstrained eigenvalues)
```

Model Building

- The `$anova` component contains a summary of the steps involved in automatic model building

```
> mods$anova
```

```
  Step Df Deviance Resid. Df Resid. Dev      AIC
1      NA       NA        23   5036.590 130.3143
2 + Al -1 720.9014        22   4315.689 128.6070
3  + P -1 459.1399        21   3856.549 127.9074
4  + K -1 377.2927        20   3479.256 127.4365
```

Model Building

- Step-wise model selection is fairly fragile; if we start from the full model we won't end up with the same final model

```
> mods2 <- step(upr, scope = list(lower = formula(lwr), upper = formula(upr)), trace = 0,
+               test = "perm")
> mods2

Call: cca(formula = varespec ~ P + K + Mg + S + Mn + Mo + Baresoil +
Humdepth, data = varechem)

              Inertia Proportion Rank
Total          2.0832     1.0000
Constrained    1.1165     0.5360    8
Unconstrained  0.9667     0.4640   15
Inertia is mean squared contingency coefficient

Eigenvalues for constrained axes:
  CCA1   CCA2   CCA3   CCA4   CCA5   CCA6   CCA7   CCA8
0.4007 0.2488 0.1488 0.1266 0.0875 0.0661 0.0250 0.0130

Eigenvalues for unconstrained axes:
    CA1     CA2     CA3     CA4     CA5     CA6     CA7     CA8     CA9    CA10
0.25821 0.18813 0.11927 0.10204 0.08791 0.06085 0.04461 0.02782 0.02691 0.01646
   CA11    CA12    CA13    CA14    CA15
0.01364 0.00823 0.00655 0.00365 0.00238
```

Model Building

- The $anova component contains a summary of the steps involved in automatic model building

```
> mods2$anova

  Step Df Deviance Resid. Df Resid. Dev      AIC
1      NA       NA         9   1551.483 130.0539
2 - Fe  1 115.2085        10   1666.692 129.7730
3 - Al  1 105.9602        11   1772.652 129.2523
4  - N  1 117.5382        12   1890.190 128.7931
5 - pH  1 140.4399        13   2030.630 128.5131
6 - Ca  1 141.2450        14   2171.875 128.1270
7 - Zn  1 165.2596        15   2337.135 127.8871
```

Permutation tests — the `anova()` method

- We have little good theory with which to evaluate the significance of ordination models or terms therein
- Instead we use permutation tests
  - If there are no conditioning variables then the species data are shuffled
  - If there are constraining variables then two options are possible, both permute residuals of model fits
    - ★ Full model; residuals from the model $Y = X + Z + \varepsilon$
    - ★ Reduced model; residuals from the model $Y = Z + \varepsilon$
  - These two essentially produce the same results
- In vegan these are achieved via the `method` argument using `"direct"`, `"full"`, `"reduced"`.
- A test statistic is required; vegan uses a pseudo-F statistics

$$F = \frac{\chi^2_{model} / df_{model}}{\chi^2_{resid} / df_{resid}}$$

- Evaluate whether F is unusually large relative to the null (permutation) distribution of F

Permutation tests — the anova() method

- The main user function is the `anova()` method
- It is an interface to the lower-level function `permutest.cca()`
- At its most simplest, the `anova()` method tests whether the “model” as a whole is significant

$$F = \frac{1.4415/14}{0.6417/9} = 1.4441$$

```
> set.seed(42)
> anova(cca1)

Permutation test for cca under reduced model

Model: cca(formula = varespec ~ N + P + K + Ca + Mg + S + Al + Fe + Mn + Zn + Mo +
         Df  Chisq      F N.Perm  Pr(>F)
Model    14 1.4415 1.4441   1599 0.03562 *
Residual  9 0.6417
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
```

Permutation tests — the `anova()` method

- `anova()` will continue permuting only as long as it is uncertain whether the the p-value is above or below the chosen threshold (say $p = 0.05$)
- If the function is sure the permuted p is above the threshold `anova()` may return after only a few hundred permutations
- In other cases many hundreds or thousands of permutations may be required to say whether the model is above or below the threshold
- In the example, 1599 permutations were required

Permutation tests — the anova() method

- anova.cca() has a number of arguments

```
> args(anova.cca)

function (object, alpha = 0.05, beta = 0.01, step = 100, perm.max = 9999,
    by = NULL, ...)
NULL
```

- alpha is the desired p value threshold (Type I)
- beta is the Type II error rate
- Permuting stops if the result is different from alpha for the given beta
- This is evaluated every step permutations
- perm.max sets a limit on the number of permutations
- by determines what is tested; the default is to test the model
- More direct control can be achieved via permutest.cca()

Permutation tests — testing canonical axes

- The canonical axes can be individually tested by specifying `by = "axis"`
- The first axis is tested in terms of variance explained compared to residual variance
- The second axis is tested after partialling out the first axis, ...

```
> set.seed(1)
> anova(mods, by = "axis")

Model: cca(formula = varespec ~ Al + P + K, data = varechem)
         Df  Chisq      F N.Perm  Pr(>F)
CCA1      1 0.3616 5.0249    199 0.00500 **
CCA2      1 0.1700 2.3621    299 0.01667 *
CCA3      1 0.1126 1.5651     99 0.16000
Residual 20 1.4391
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
```

Permutation tests — testing terms

- The individual terms in the model can be tested using `by = "terms"`
- The terms are assessed in the order they were specified in the model, sequentially from first to last
- It is important to note that the order of the terms will affect the results

```
> set.seed(5)
> anova(mods, by = "terms")

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

Model: cca(formula = varespec ~ Al + P + K, data = varechem)
         Df  Chisq      F N.Perm Pr(>F)
Al        1 0.2982 4.1440     99   0.01 **
P         1 0.1899 2.6393     99   0.01 **
K         1 0.1561 2.1688     99   0.03 *
Residual 20 1.4391
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Permutation tests — testing marginal terms

- The marginal "effect" of a model term can be assessed using `by = "margin"`
- The marginal "effect" is the effect of a particular term when all other model terms are included in the model

```
> set.seed(5)
> anova(mods, by = "margin")

Permutation test for cca under reduced model
Marginal effects of terms

Model: cca(formula = varespec ~ Al + P + K, data = varechem)
         Df  Chisq      F N.Perm Pr(>F)
Al        1 0.3118 4.3340    199  0.005 **
P         1 0.1681 2.3362    199  0.010 **
K         1 0.1561 2.1688    399  0.020 *
Residual 20 1.4391
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
```

Diagnostics for constrained ordination

- Vegan provides a series of diagnostics functions to help assess the model fit
- `goodness()` computes two goodness of fit statistics for species or sites
  - `statistic = "explained"` — cumulative proportion of variance explained by each axis
  - `statistic = "distance"` — the residual distance between the "fitted" location in ordination space and the full dimensional space
- `inertiacomp()` decomposes the variance for each species or site into partial, constrained and unexplained components
- `intersetcor()` computes the interset correlations, the (weighted) correlation between the weighted average site scores and the linear combination site scores
- `vif.cca()` computes variance inflation factors for model constrains. Variables with $V > 10$ are linearly dependent on other variables in the model

Linear methods

- Vegan can also fit the linear methods PCA and RDA
- Linear based ordination methods are handled in the same way as their unimodal counter parts
- The `rda()` function is used to fit these two techniques
- Interface is the same as & the object returned is as described for `cca()`
- Class `c("rda","cca")`

```
> data(dune); data(dune.env)
> (pca1 <- rda(dune, scale = TRUE))
Call: rda(X = dune, scale = TRUE)

              Inertia Rank
Total              30
Unconstrained      30   19
Inertia is correlations

Eigenvalues for unconstrained axes:
  PC1   PC2   PC3   PC4   PC5   PC6   PC7   PC8
7.032 4.997 3.555 2.644 2.139 1.758 1.478 1.316
(Showed only 8 of all 19 unconstrained eigenvalues)
```

Linear methods

- The `scale` argument controls whether the response data are standardised prior to analysis. Vegan always performs a centred PCA/RDA

```
> (rda1 <- rda(dune ~ Manure, dune.env, scale = TRUE))

Call: rda(formula = dune ~ Manure, data = dune.env, scale = TRUE)

              Inertia Proportion Rank
Total         30.0000     1.0000     
Constrained    8.7974     0.2932    4
Unconstrained 21.2026     0.7068   15
Inertia is correlations 

Eigenvalues for constrained axes:
 RDA1  RDA2  RDA3  RDA4 
4.374 2.078 1.449 0.896 

Eigenvalues for unconstrained axes:
  PC1   PC2   PC3   PC4   PC5   PC6   PC7   PC8   PC9  PC10  PC11  PC12  PC13 
5.133 3.447 2.462 1.924 1.662 1.366 1.357 0.926 0.839 0.585 0.511 0.439 0.308 
 PC14  PC15 
0.159 0.084 
```

Outline

Dissimilarities

- `dist()` is the basic R function for computing dissimilarity or distance matrices
- Few, if any, of the included metrics are suitable for community ecology data
- Vegan provides `vegdist()` as a drop-in alternative with numerous useful metrics
  - Bray-Curtis
  - Jaccard
  - Gower
  - Kulczynski
  - Give good gradient separation for ecological data
- Returns an object of class `"dist"` which can be used in many other R functions & packages

```
> dis <- vegdist(varespec, method = "bray")
> dis2 <- vegdist(varespec, method = "gower")
> class(dis)

[1] "dist"
```

Ecologically meaningful transformations

- Legendre & Gallagher (Oecologia, 2001) show that many ecologically useful dissimilarities are in Euclidean form
- They are equivalent to calculating the Euclidean distance on **transformed** data
- Two of the suggested metrics included in vegan's `decostand()` function
  - Chi-square
  - Hellinger

```
> dis3 <- vegdist(decostand(varespec, method = "hellinger"))
```

Principal coordinates analysis

- Principal Coordinates Analysis (PCoA) (AKA classic or metric multidimensional scaling) is PCA applied to a dissimilarity matrix
- Several functions in R available for this (e.g. `cmdscale()`)
- Vegan has `capscale()` for constrained analysis of principal coordinates (CAP)
- Works exactly the same way as `rda()`
- Can supply a dissimilarity matrix as the response or the community data and tell vegan which dissimilarity to compute
- Several new arguments
  - `distance` & `dfun` indicate which dissimilarity to compute and which function to use to compute it
  - `sqrt.dist` & `add` allow handling of negative λ (not needed but can be used)
  - `comm` the community data is a dissimilarity matrix used in the model formula; allows species scores to be added
  - `metaMDSdist` process the community data before analysis using `metaMDSdist()`; allows transformations & extended dissimilarities

Principal coordinates analysis

- To use `capscale()` for PCoA provide a formula with an intercept only
- LHS of formula is community data or dissimilarity matrix

```
> (pcoa <- capscale(varespec ~ 1, dist = "bray", metaMDS = TRUE))

Square root transformation
Wisconsin double standardization
Call: capscale(formula = varespec ~ 1, distance = "bray", metaMDSdist =
TRUE)

               Inertia Rank
Total          2.54753     
Real Total     2.59500     
Unconstrained  2.59500   19
Imaginary     -0.04747    4
Inertia is squared Bray distance

Eigenvalues for unconstrained axes:
  MDS1   MDS2   MDS3   MDS4   MDS5   MDS6   MDS7   MDS8
0.6075 0.3820 0.3335 0.2046 0.1731 0.1684 0.1505 0.1163
(Showed only 8 of all 19 unconstrained eigenvalues)

metaMDSdist transformed data: wisconsin(sqrt(varespec))

> class(pcoa)

[1] "capscale" "rda"      "cca"
```

Constrained Principal coordinates analysis

- Constrained Analysis of Principal Coordinates (CAP)
- Constrained form of PCoA (as RDA is to PCA, CCA is to CA, etc.)
- Similar to CAP of Anderson & Willis (2003, *Ecology* 84, 511–525) but with a couple of enhancements
  - Uses PCoA axes weighted by λ_i so ordination distances best approximate the original dissimilarities (CAP uses orthonormal PCoA axes; noise!)
  - CAP uses a subset of axes, `capscale()` uses all real PCoA axes
  - `capscale()` adds species scores as weighted sums of community data

Constrained Principal coordinates analysis

- Constrained Analysis of Principal Coordinates (CAP)

```
> (vare.cap <- capscale(varespec ~ N + P + K + Condition(Al), varechem,
+                       dist = "bray"))

Call: capscale(formula = varespec ~ N + P + K + Condition(Al), data =
varechem, distance = "bray")

              Inertia Proportion Rank
Total          4.5444
Real Total     4.8034     1.0000
Conditional    0.9772     0.2034    1
Constrained    0.9972     0.2076    3
Unconstrained  2.8290     0.5890   15
Imaginary     -0.2590               8
Inertia is squared Bray distance

Eigenvalues for constrained axes:
  CAP1   CAP2   CAP3
0.5413 0.3265 0.1293

Eigenvalues for unconstrained axes:
  MDS1   MDS2   MDS3   MDS4   MDS5   MDS6   MDS7   MDS8   MDS9  MDS10  MDS11
0.9065 0.5127 0.3379 0.2626 0.2032 0.1618 0.1242 0.0856 0.0689 0.0583 0.0501
 MDS12  MDS13  MDS14  MDS15
0.0277 0.0208 0.0073 0.0013
```

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

```
> library("vegan"); data(dune)
> set.seed(42)
> (sol <- metaMDS(dune))

Run 0 stress 0.1192678
Run 1 stress 0.1183186
... New best solution
... procrustes: rmse 0.02026936  max resid 0.06495232
Run 2 stress 0.1192678
Run 3 stress 0.1183186
... procrustes: rmse 5.509367e-06  max resid 1.511849e-05
*** Solution reached

Call:
metaMDS(comm = dune)

global Multidimensional Scaling using monoMDS

Data:     dune
Distance: bray

Dimensions: 2
Stress:     0.1183186
Stress type 1, weak ties
Two convergent solutions found after 3 tries
Scaling: centring, PC rotation, halfchange scaling
Species: expanded scores based on ‘dune’
```

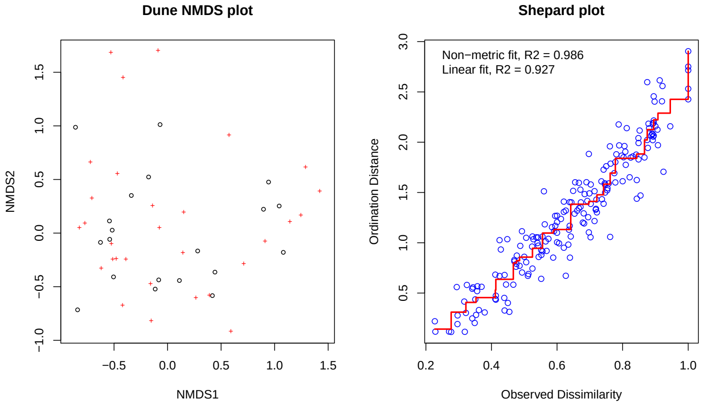
NMDS in vegan

- If no convergent solutions, continue iterations from previous best solution

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

Starting from 2-dimensional configuration
Run 0 stress 0.1183186
Run 1 stress 0.1183186
... procrustes: rmse 1.919781e-05  max resid 6.3831e-05
*** Solution reached

Call:
metaMDS(comm = dune, 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 4 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)
```


Dune NMDS plot
NMDS1
NMDS2
Shepard plot
Non−metric fit, R2 = 0.986
Linear fit, R2 = 0.927
Observed Dissimilarity
Ordination Distance