A (brief) introduction to ordination and the vegan package

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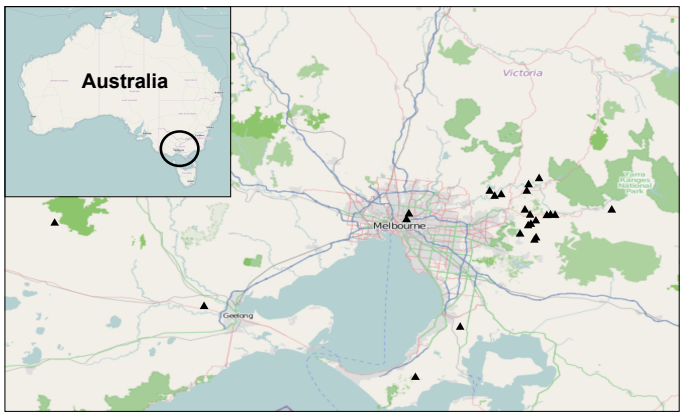
SEFS9, July 5th 2015

Datasets

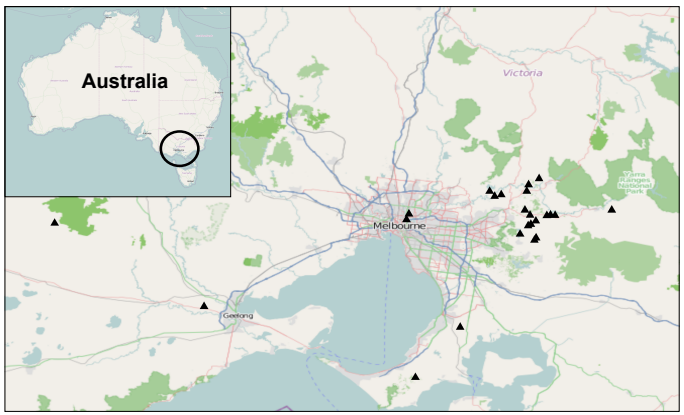
Exercise: Salinization and Pestices



- Macroivertebrates
- 24 sites
- covering a salinity and toxicity gradient

The dataset is published in: Szöcs, E., Kefford, B.J., Schäfer, R.B., 2012. Is there an interaction of the effects of salinity and pesticides on the community structure of macroinvertebrates? Science of the Total Environment 437, 121–126.

Exercise: Salinization and Pestices



- Macroivertebrates
- 24 sites
- covering a salinity and toxicity gradient

Questions:

- Interaction between salinization and pesticides?
- Which species are affected?
- Other influences?

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Exercise: Salinization and Pestices

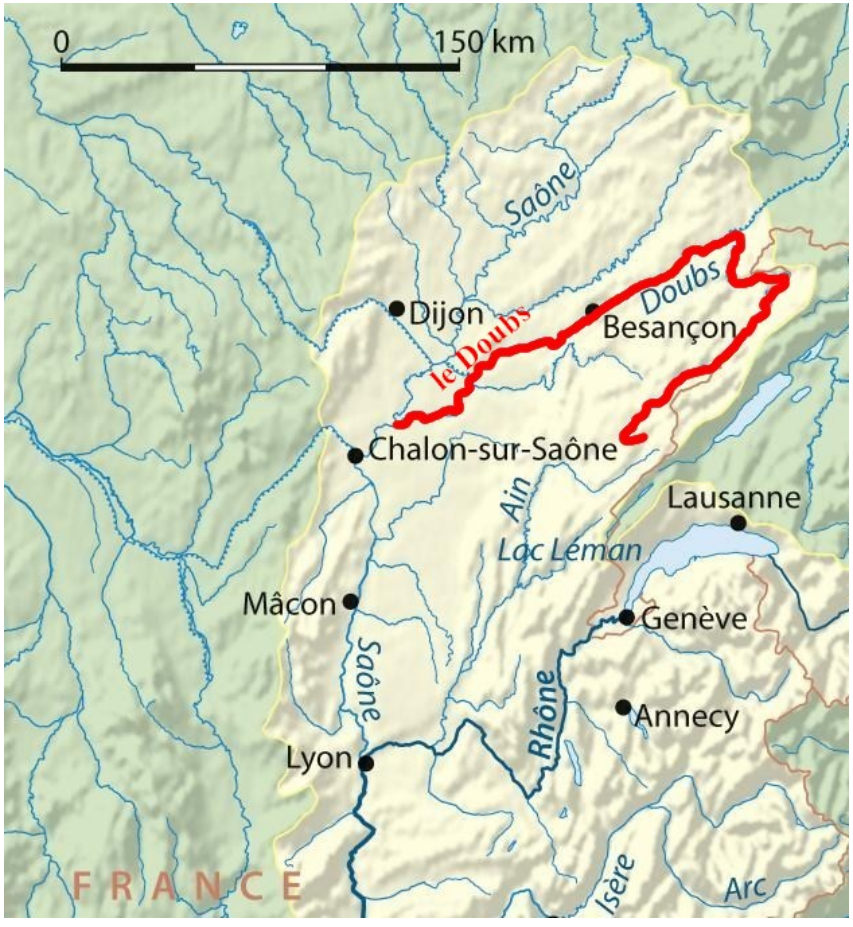
```
setwd('yourpath/3-IntroVeganPackage/data/')
abu <- read.table('melbourneAbu.csv', sep = ';', header = TRUE)
env <- read.table('melbourneEnv.csv', sep = ';', header = TRUE)
```

```
dim(env)

[1] 24 23

dim(abu)

[1] 24 76
```

24 sites, 22 environmental variables, 75 taxa

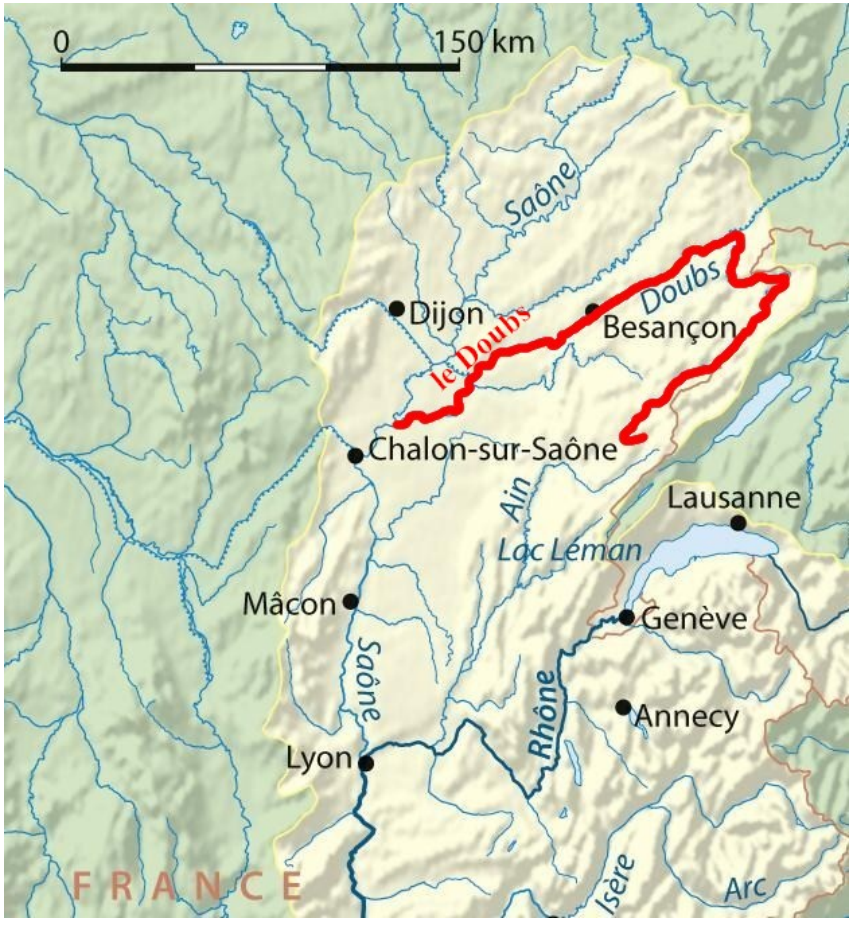
```
head(env[ , 1:10])

    ID    T   pH oxygen Depth maxwidth minwidth rifperc poolperc Bedrock
1 1-11 16.8 7.67   80.1   0.9       15     12.0       0      100       0
2 2-11 16.5 7.29   83.0   0.9       30     15.0       0      100       0
3 3-11 17.3 7.20   77.9   0.4        4      2.5       0      100       0
4 4-11 15.6 7.84   72.0   0.7        8      2.5       0      100       0
5 5-11 17.2 6.97   69.9   0.9        7      4.0       0      100       0
6 6-11 15.5 7.26   80.0   0.2        3      2.0       5       95       0
```

Demonstration: Doubs river fish communities



- Fish
- 30 sites along the Doubs River

Demonstration: Doubs river fish communities



- Fish
- 30 sites along the Doubs River

Questions

- How does fish composition change downstream?
- Environmental drivers?

Demonstration: Doubs river fish communities — Species

```
setwd('your/workingdirectory')
Dabu <- read.table('doubsAbu.csv', sep = ',', header = TRUE)
Denv <- read.table('doubsEnv.csv', sep = ',', header = TRUE)
Dspa <- read.table('doubsSpa.csv', sep = ',', header = TRUE)
```

```
dim(Dabu)

[1] 30 27
```

30 sites, 27 taxa

```
head(Dabu[ , 1:18])

  CHA TRU VAI LOC OMB BLA HOT TOX VAN CHE BAR SPI GOU BRO PER BOU PSO ROT
1   0   3   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0
2   0   5   4   3   0   0   0   0   0   0   0   0   0   0   0   0   0   0
3   0   5   5   5   0   0   0   0   0   0   0   0   0   1   0   0   0   0
4   0   4   5   5   0   0   0   0   0   1   0   0   1   2   2   0   0   0
5   0   2   3   2   0   0   0   0   5   2   0   0   2   4   4   0   0   2
6   0   3   4   5   0   0   0   0   1   2   0   0   1   1   1   0   0   0
```

Demonstration: Doubs river fish communities — Environment

```
dim(Denv)

[1] 30 11
```

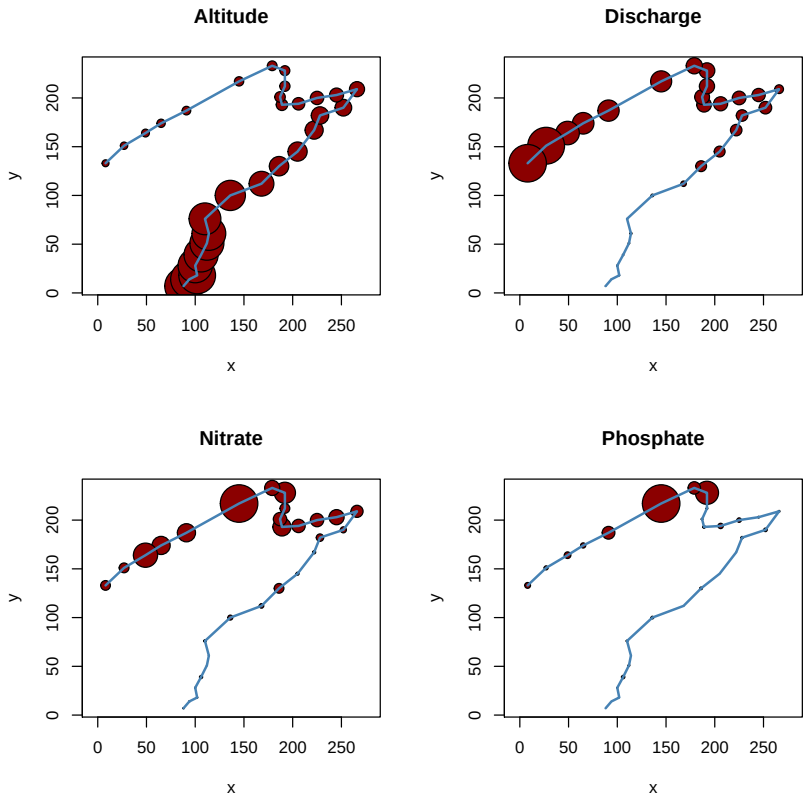
30 sites, 11 variables

```
head(Denv)

   das alt  pen  deb  pH dur  pho  nit  amm  oxy dbo
1  0.3 934 48.0 0.84 7.9  45 0.01 0.20 0.00 12.2 2.7
2  2.2 932  3.0 1.00 8.0  40 0.02 0.20 0.10 10.3 1.9
3 10.2 914  3.7 1.80 8.3  52 0.05 0.22 0.05 10.5 3.5
4 18.5 854  3.2 2.53 8.0  72 0.10 0.21 0.00 11.0 1.3
5 21.5 849  2.3 2.64 8.1  84 0.38 0.52 0.20  8.0 6.2
6 32.4 846  3.2 2.86 7.9  60 0.20 0.15 0.00 10.2 5.3
```

Unconstrained Ordination

Principal Components Analysis (PCA)
Principal coordinates analysis (PCoA)
Nonmetric Multidimensional Scaling (NMDS)

Principal Components Analysis (PCA) — Why?

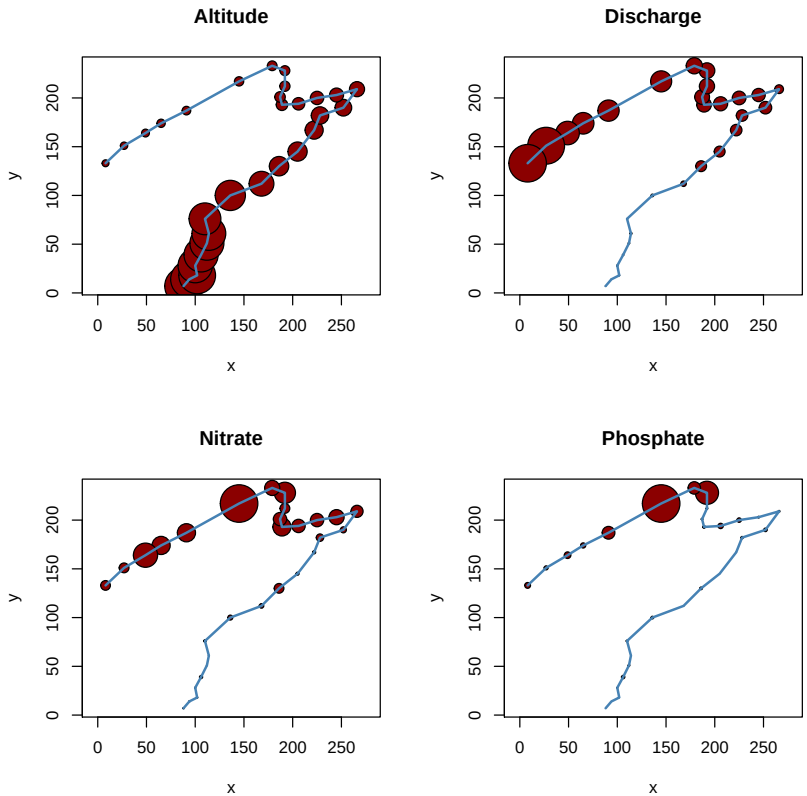


- 11 variables

Questions:

- Which variable are correlated?
- Which sites have similar conditions?
- How do conditions change downstream?

Principal Components Analysis (PCA) — Why?



- 11 variables

Questions:

- Which variable are correlated?
- Which sites have similar conditions?
- How do conditions change downstream?

- pairwise comparisons
- 3D possible
- more than 3 dimensions?

Principal Components Analysis (PCA) — What?

- *"Look from another angle on the data"*
- PCA is just a rotation of the coordinate system
- The rotation is done so that the first axis contains as much variation as possible
- Second axis than most of remaining variation

Principal Components Analysis (PCA) — What?

- *"Look from another angle on the data"*
- PCA is just a rotation of the coordinate system
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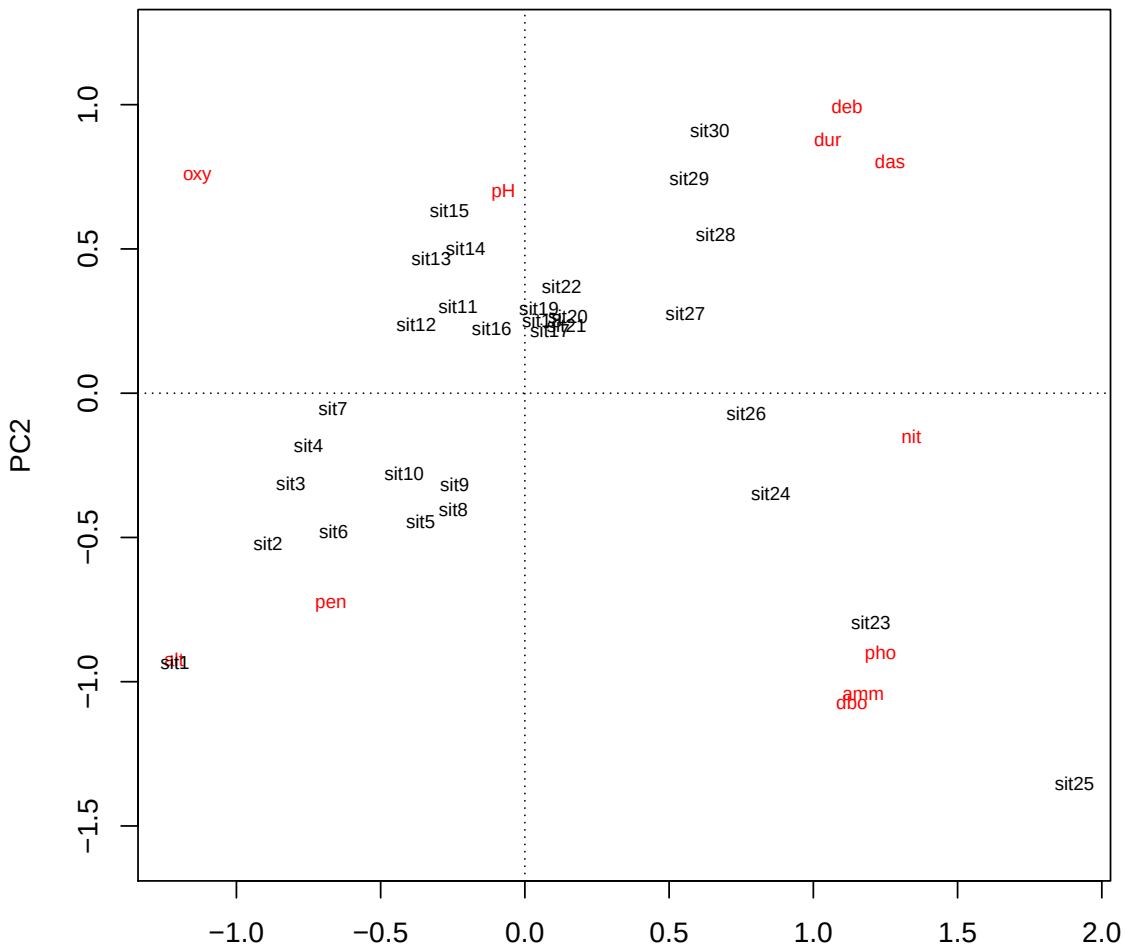
Maths:

- The covariance (or correlation) matrix is decomposed into its Eigenvectors and Eigenvalues.
- The Eigenvectors give the roration needed
- The Eigenvalues stretch the axes

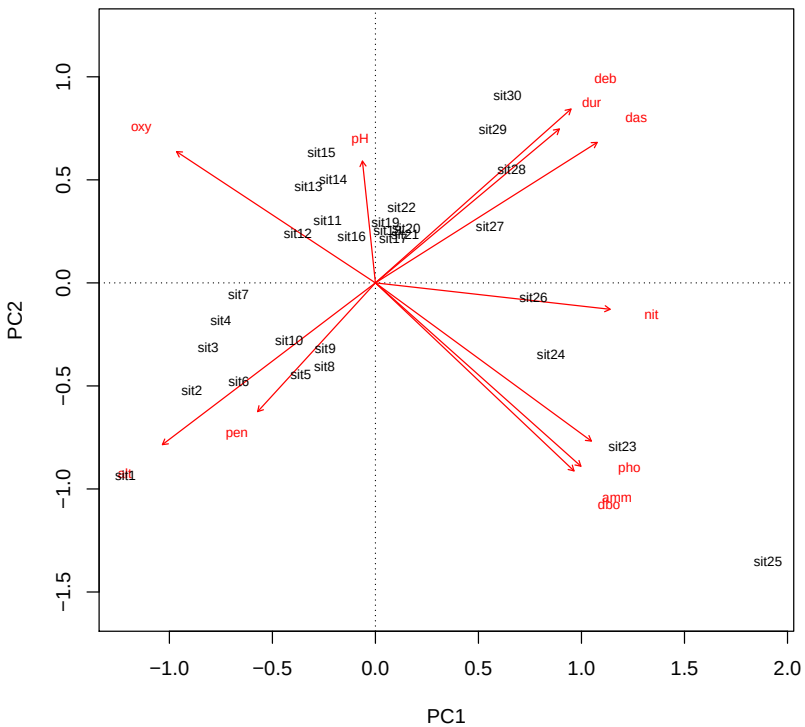
Principal Components Analysis (PCA) — How?

```
require(vegan)
PCA <- rda(Denv, scale = TRUE)
plot(PCA, scaling = 3)
```



Principal Components Analysis (PCA) — Interpretation? (I)

```
biplot(PCA, cex = 5, scaling = 3)
```



Principal Components Analysis (PCA) — Interpretation? (II)

```
summary(PCA, display = NULL, scaling = 3)
```

```
Call:
rda(X = Denv, scale = TRUE)

Partitioning of correlations:
              Inertia Proportion
Total              11          1
Unconstrained      11          1

Eigenvalues, and their contribution to the correlations

Importance of components:
                          PC1    PC2     PC3     PC4     PC5     PC6    PC7
Eigenvalue             5.9687 2.1638 1.06516 0.73873 0.40027 0.33565 0.1727
Proportion Explained   0.5426 0.1967 0.09683 0.06716 0.03639 0.03051 0.0157
Cumulative Proportion  0.5426 0.7393 0.83616 0.90331 0.93970 0.97022 0.9859
                           PC8     PC9    PC10     PC11
Eigenvalue             0.10821 0.02368 0.01707 0.005993
Proportion Explained   0.00984 0.00215 0.00155 0.000540
Cumulative Proportion  0.99575 0.99790 0.99946 1.000000

Scaling 3 for species and site scores
* Both sites and species are scaled proportional to eigenvalues
 on all dimensions
* General scaling constant of scores:
```

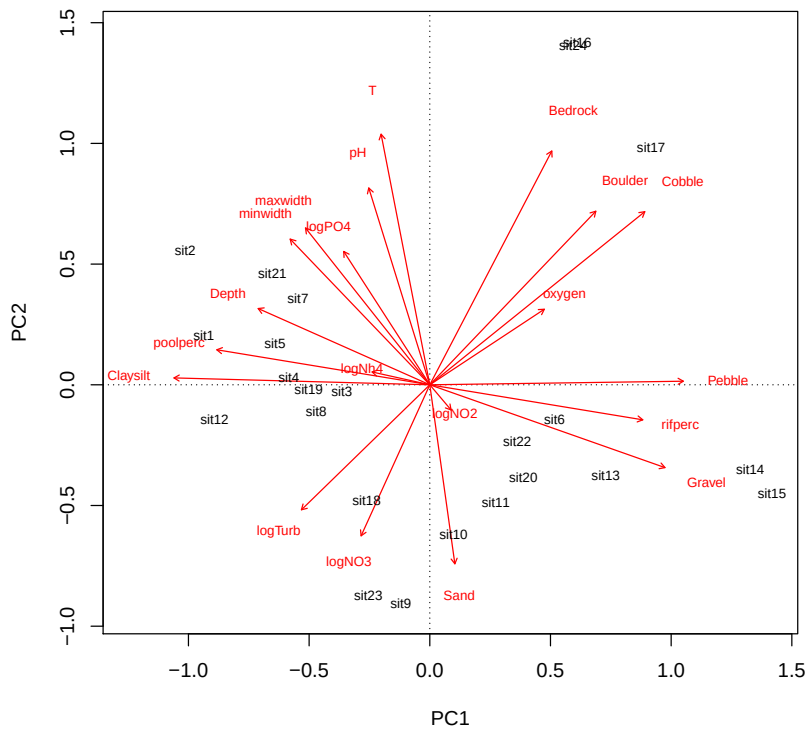
Your turn!

Load the Melbourne dataset (only environmental variables).
Exclude the variables ID, logCond and logmaxTU.
Perform a PCA.
Which variables are correlated?
What other gradients are present in this dataset?

Exercise

```
take <- env[ , !names(env) %in% c('ID', 'logCond', 'logmaxTU')]
PCA <- rda(take, scale = TRUE)
```

```
biplot(PCA, scaling = 3)
```



- multiple variables interrelated
- 1st axis can be intepreted as *hydrological gradient*
- 2nd axis can be intepreted as *chemistry gradient*

Excursus — principal component regression (PCR)

Question:

- How is diversity related to salinity, pesticides and other variables?

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Problem:

- Only 24 sites
- but 22 (partly correlated) explanatory variables
- strongy hypotheses about salinity and pesticides

A Solution:

Excursus — principal component regression (PCR)

Question:

- How is diversity related to salinity, pesticides and other variables?

Problem:

- Only 24 sites
- but 22 (partly correlated) explanatory variables
- strongy hypotheses about salinity and pesticides

A Solution:

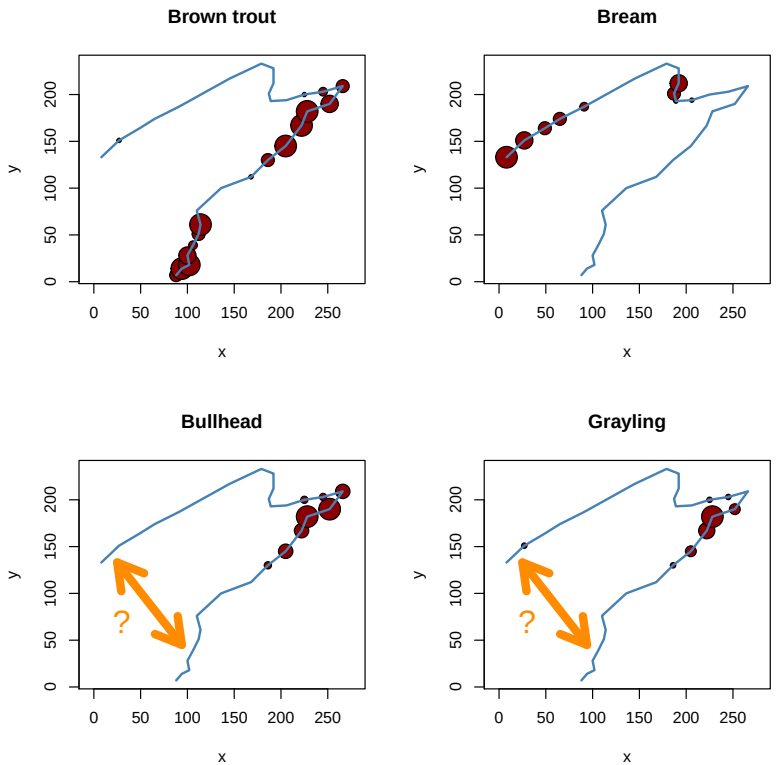
- Reduce number of variables to *Principal Components*
- regress these

Excursus — principal component regression (PCR)

```r
div <- diversity(abu[ , -1], index = 'shannon')
pc <- scores(PCA, choices = c(1, 2), scaling = 1, display = 'sites')
model_data <- data.frame(div, pc, logCond = env$logCond, logmaxTU = env$logmaxTU)
model <- lm(div ~ PC1 + PC2 + logCond + logmaxTU, data = model_data)
summary(model)
```

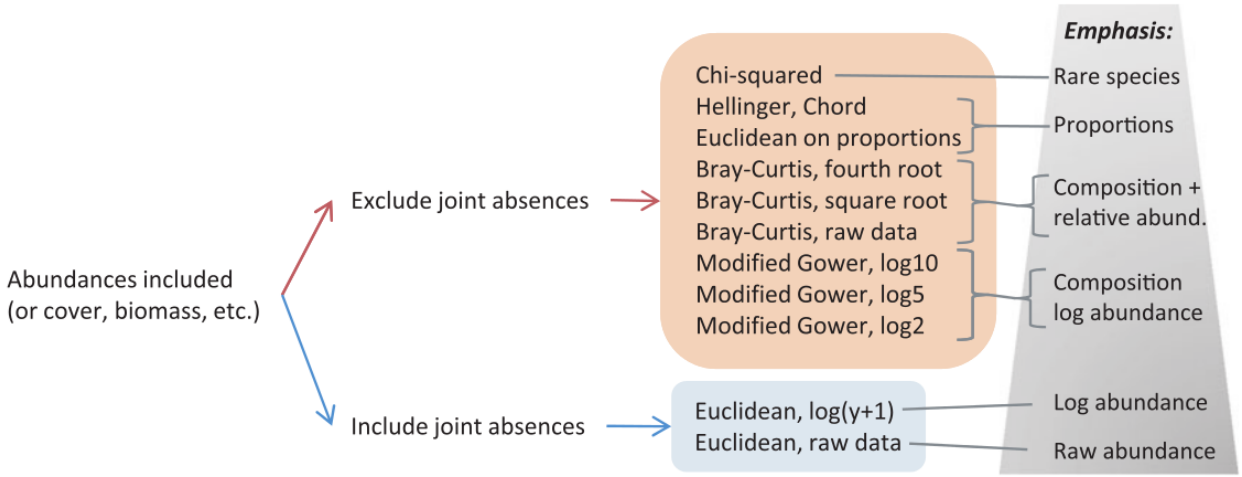
```
Call:
lm(formula = div ~ PC1 + PC2 + logCond + logmaxTU, data = model_data)

Residuals:
     Min       1Q   Median       3Q      Max
-0.64415 -0.15688  0.02063  0.18219  0.57929

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  1.83079    0.43429   4.216 0.000468 ***
PC1          0.01971    0.16691   0.118 0.907262
PC2          0.02192    0.19570   0.112 0.911996
logCond     -0.20942    0.13050  -1.605 0.125049
logmaxTU    -0.12572    0.07316  -1.718 0.101994
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.3645 on 19 degrees of freedom
Multiple R-squared:  0.2682, Adjusted R-squared:  0.1141
F-statistic: 1.741 on 4 and 19 DF,  p-value: 0.1827
```

Abundances — The Problem with zeros



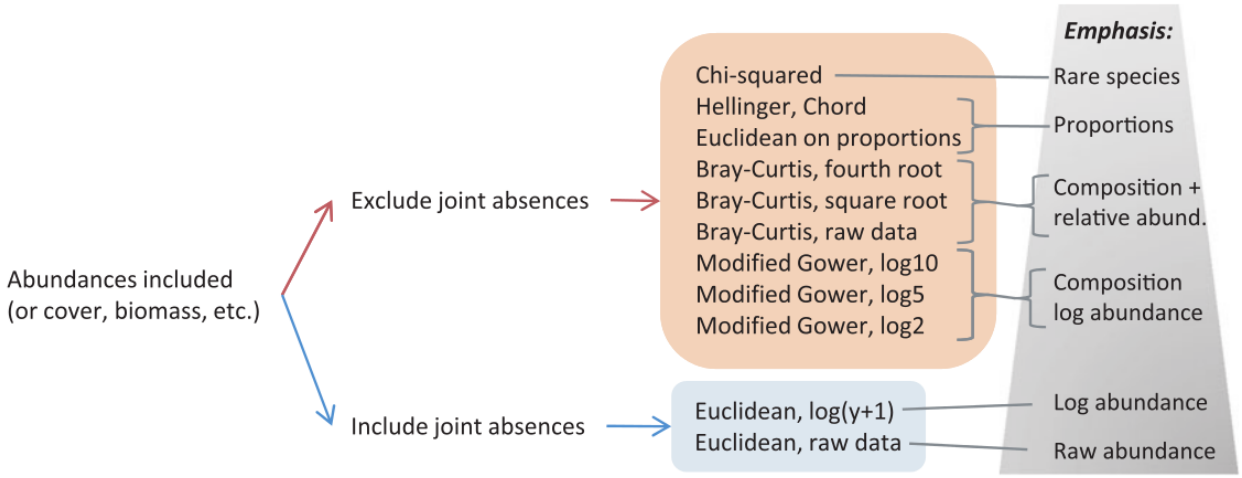
- Species may be absent due to different factors (too high flow, too saline, etc.)
- *Absence* contains less information then *Presence*
- PCA preserves the euclidean distance between sites
- Need another measure of similarity for (raw) abundances

Dissimilarity measures



Anderson, M.J., Crist, T.O., et al. , 2011. Navigating the multiple meanings of beta diversity: a roadmap for the practicing ecologist. Ecology Letters 14, 19–28.

Dissimilarity measures




```
     Spe1 Spe2 Spe3
sit1    0    4    8
sit2    0    1    1
sit3    1    0    0
```

```
vegdist(mat, method = 'euclidean')
```

```
         1        2
2 7.615773
3 9.000000 1.732051
```

```
vegdist(mat, method = 'bray')
```

```
           1         2
2 0.7142857
3 1.0000000 1.0000000
```

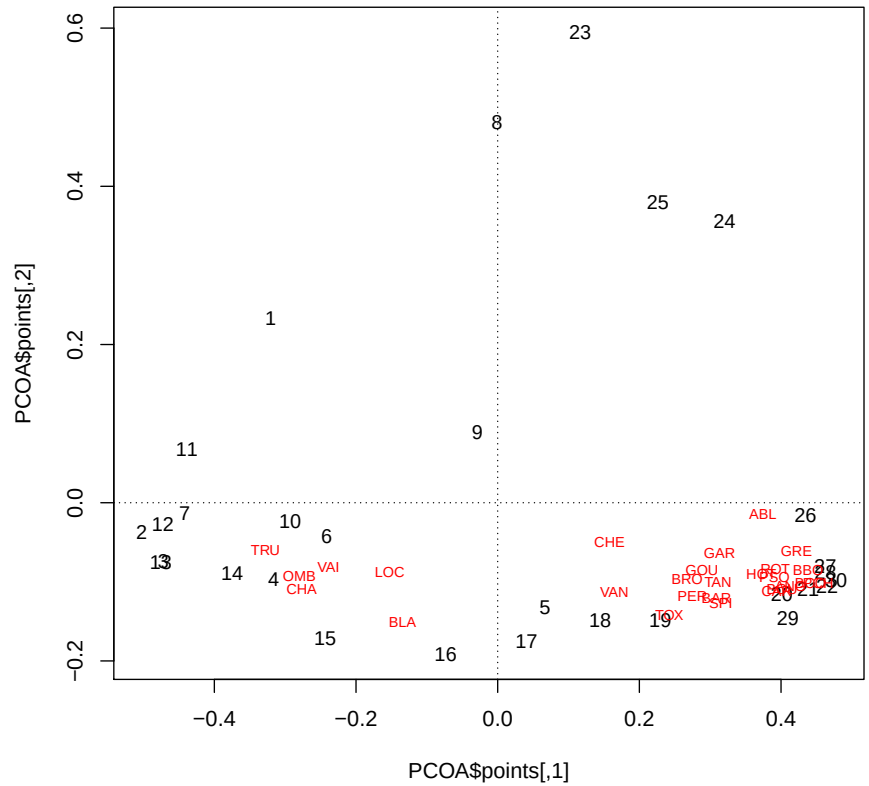
Anderson, M.J., Crist, T.O., et al. , 2011. Navigating the multiple meanings of beta diversity: a roadmap for the practicing ecologist. Ecology Letters 14, 19–28.

Principal coordinates analysis (PCoA)

- Works on distance matrices
- Species can be added as *weighted averages*
- Eigenvalue based
- PCoA with euclidean distance == PCA

Principal coordinates analysis (PCoA)

```r
# Distance matrix
Dabu_dist <- vegdist(Dabu, method = 'bray')

# PCoA
PCOA <- cmdscale(Dabu_dist, eig = TRUE)

# Create plot
plot(PCOA$points, type = 'n')
text(PCOA$points,
     labels = rownames(Dabu), cex = 0.9)
abline(h = 0 , lty = 'dotted')
abline(v = 0 , lty = 'dotted')

# Add species as weighted averages
wa <- wascores(PCOA$points, Dabu)
text(wa, labels = colnames(Dabu),
     col = 'red', cex = 0.7)
```



Nonmetric Multidimensional Scaling (NMDS)

Your turn!

Using the melbourne data.

Indirect Gradient Analysis

Your turn!

Using the melbourne data.

Constrained Ordination

Constrained Ordination

- Redundany analysis (RDA)
- Transformation-based RDA
- Distance-based RDA

Your turn!

Using the melbourne data.

Permutation Tests

Your turn!

Using the melbourne data.