Training in ade4 in R - Module I: Basic methods

Principal component analysis

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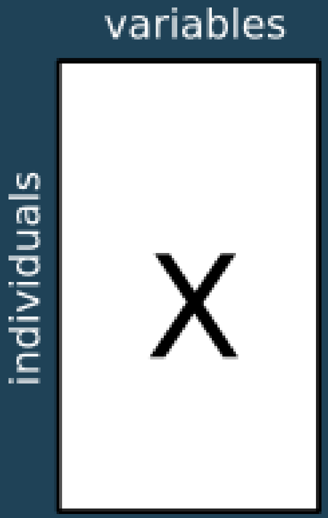
Data structure



- One table with *p* variables measured on *n* individuals
- All variables are **quantitative**
- For instance
  - sites × environmental variables
  - species × traits
  - individuals × alleles
  - populations × alleles

Objectives

- Identify what is the main information contained in the table
  - Identify which variables are the most linked
  - Identify the principal differences/similarities between individuals

Data

We consider the `meaudret` data set

```r
library(ade4)
data(meaudret)
names(meaudret)
```

```
## [1] "env"       "design"    "spe"       "spe.names"
```

```r
dim(meaudret$env)
```

```
## [1] 20  9
```

```r
names(meaudret$env)
```

```
## [1] "Temp" "Flow" "pH"   "Cond" "Bdo5" "Oxyd" "Ammo" "Nitr" "Phos"
```

The data set contains an environmental table with 20 measurements of 9 environmental variables. The measurements have been made in 6 sites at each season along a small French stream (see `?meaudret`)

```
head(meaudret$design)
```

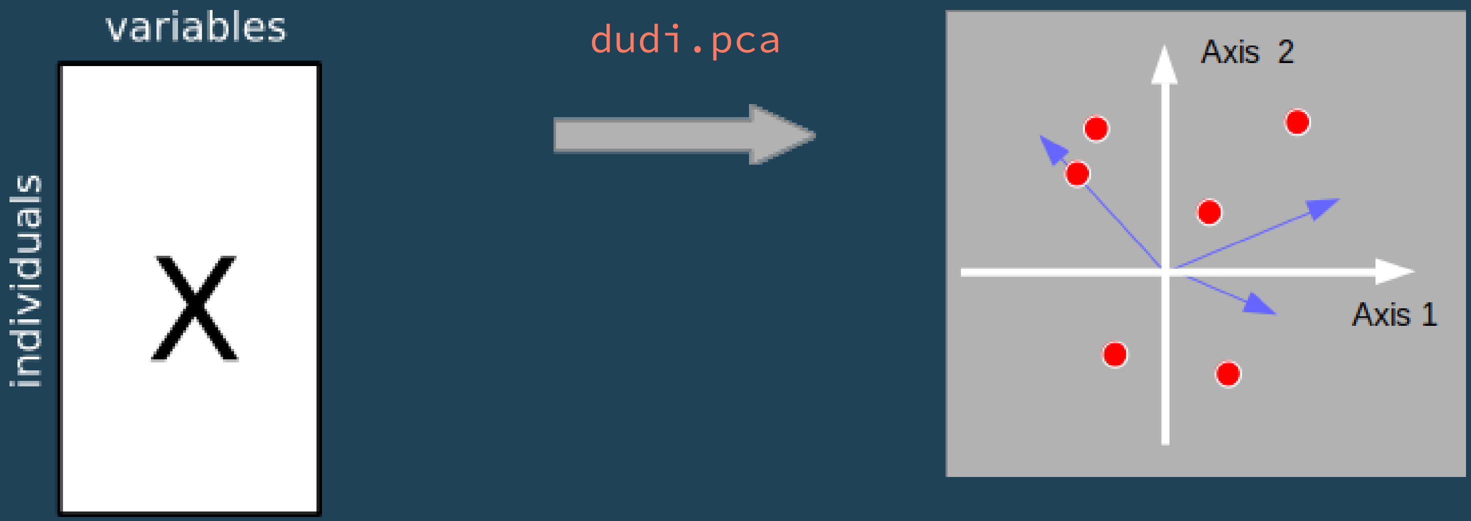
```
##      season site
## sp_1 spring   S1
## sp_2 spring   S2
## sp_3 spring   S3
## sp_4 spring   S4
## sp_5 spring   S5
## su_1 summer   S1
```

We want to know

- what are the main environmental gradients, i.e., which variables co-vary (if any)
- which samples have similar/different environmental conditions

Principal component analysis

- $\mathbf{X}$ contains centred or scaled variables
- $\mathbf{Q} = \mathbf{I}_p$ is the identity matrix (diagonal matrix with 1s)
- $\mathbf{D} = \frac{1}{n}\mathbf{I}_n$ is the diagonal matrix with $\frac{1}{n}$



`dudi.pca`

Maximized criteria

- For individuals

$$Q(\mathbf{a}) = \|\mathbf{XQa}\|^2_{\mathbf{D}} = \|\mathbf{Xa}\|^2_{\frac{1}{n}\mathbf{I}_n} = var(\mathbf{Xa}) = \lambda$$

- For variables
  - Centred data ($x_{ij} - \bar{x}_j$)

$$S(\mathbf{b}) = \|\mathbf{X}^\top\mathbf{Db}\|^2_{\mathbf{Q}} = \|\frac{1}{n}\mathbf{X}^\top\mathbf{b}\|^2_{\mathbf{I}_p} = \sum_{j=1}^{p} cov^2(\mathbf{x}_j, \mathbf{b}) = \lambda$$

  - Scaled data ($(x_{ij} - \bar{x}_j)/s_j$)

$$S(\mathbf{b}) = \|\mathbf{X}^\top\mathbf{Db}\|^2_{\mathbf{Q}} = \|\frac{1}{n}\mathbf{X}^\top\mathbf{b}\|^2_{\mathbf{I}_p} = \sum_{j=1}^{p} cor^2(\mathbf{x}_j, \mathbf{b}) = \lambda$$

The `dudi.pca` function

Arguments

```r
args(dudi.pca)
```

```
## function (df, row.w = rep(1, nrow(df))/nrow(df), col.w = rep(1, 
##     ncol(df)), center = TRUE, scale = TRUE, scannf = TRUE, nf = 2) 
## NULL
```

- `df` is a `data.frame` with the data
- `row.w` and `col.w` are optional vectors of weights
- `center` and `scale` define the standardization of the data
- `scannf` and `nf` allow to set the number of dimensions to interpret

```r
pca.meau <- dudi.pca(meaudret$env, scannf = FALSE)
```

Returned values

```r
names(pca.meau)
```

```
##  [1] "tab"  "cw"   "lw"   "eig"  "rank" "nf"   "c1"   "li"   "co"   "l1"  
## [11] "call" "cent" "norm"
```

It returns an object of class `dudi` containing:

- `$eig`: eigenvalues ($\mathbf{\Lambda}$)
- `$cw`: column weights ($\mathbf{Q} = \mathbf{I}_p$)
- `$lw`: row weights ($\mathbf{D} = \frac{1}{n}\mathbf{I}_n$)
- `$tab`: transformed data table ($\mathbf{X}$)
- `$c1`: principal axes or variable loadings ($\mathbf{A}$)
- `$li`: row scores ($\mathbf{L} = \mathbf{XA}$)
- `$l1`: principal components ($\mathbf{B}$)
- `$co`: column scores ($\mathbf{C} = \frac{1}{n}\mathbf{X}^\top\mathbf{B}$)

Graphical representation and interpretation

As we have *two* analyses (individuals and variables spaces), two representations can be defined:

- **distance biplot** where $\mathbf{A}$ and $\mathbf{L} = \mathbf{X}\mathbf{A}$ (`$c1`, `$li`) are superimposed.
- **correlation biplot** where $\mathbf{B}$ and $\mathbf{C} = \frac{1}{n}\mathbf{X}^\top\mathbf{B}$ (`$l1`, `$co`) are superimposed.

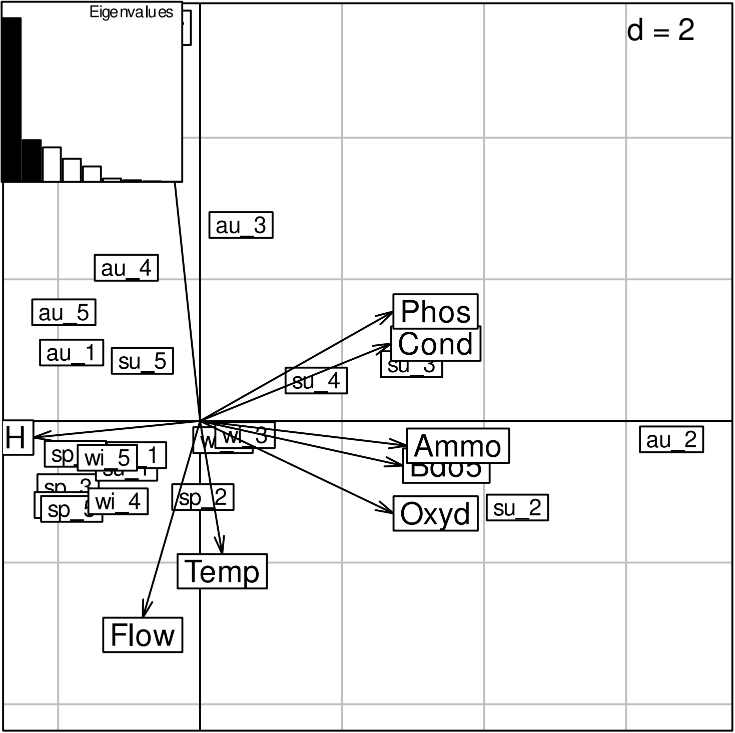
In the first interpretation, PCA finds coefficients for variables (`$c1`) to compute a linear combination (`$li`) that provides an ordination of individuals with the greatest dispersion (maximum variance).

In the second interpretation, PCA provides a linear combination (`$l1`) that maximise the correlations (`$co`) with all variables (or covariances for centred PCA). Hence, it is the best summary of the variables.

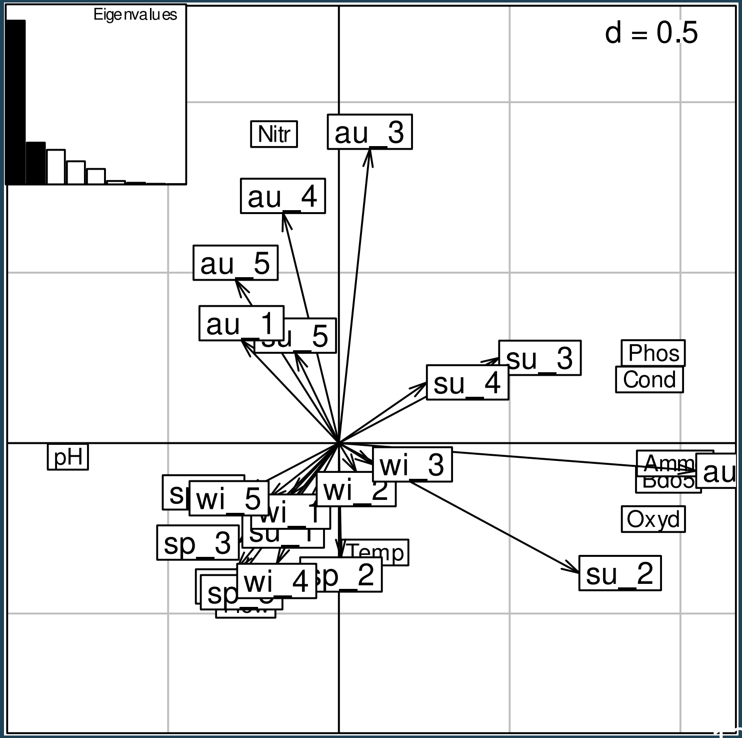
The `biplot` function

```r
library(adegraphics)
```

```r
biplot(pca.meau)
```

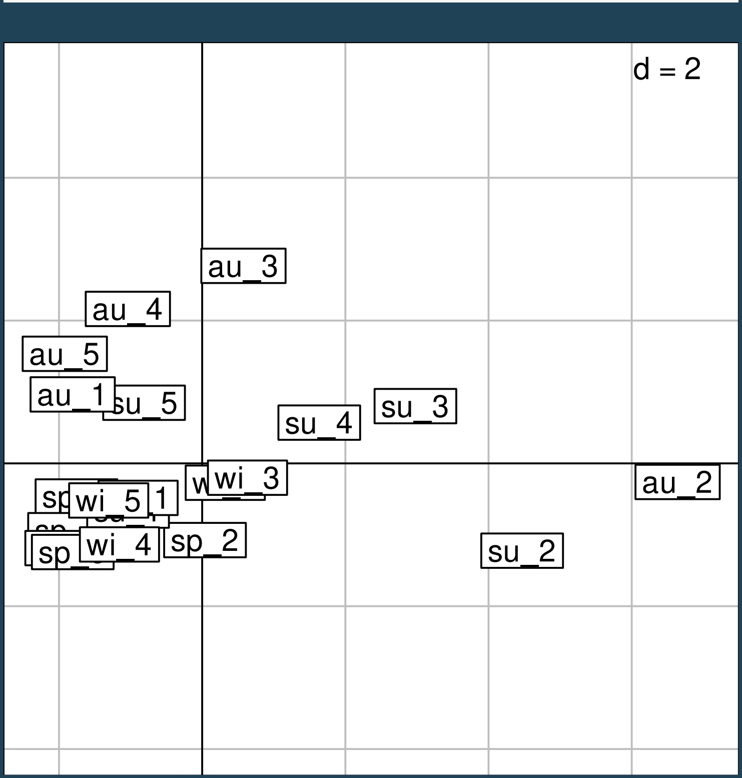


```r
biplot(pca.meau, permute = TRUE)
```

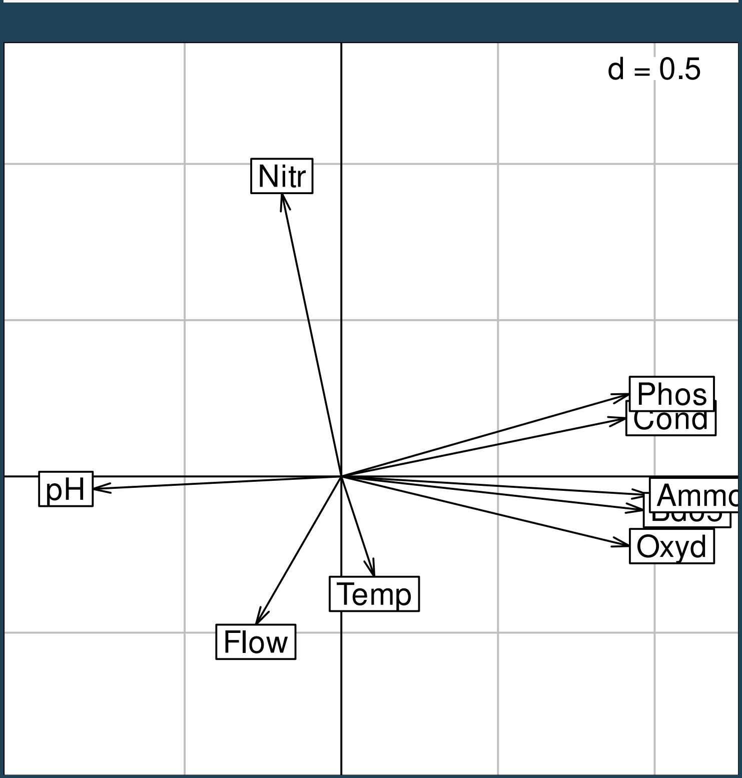


Separate representations

```
s.label(pca.meau$li)
```

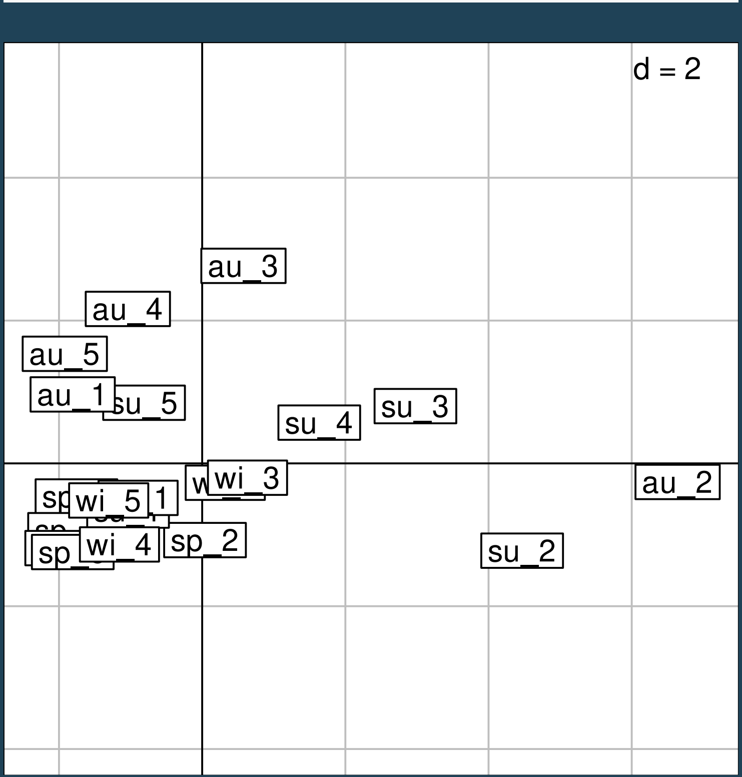


```
s.arrow(pca.meau$co)
```

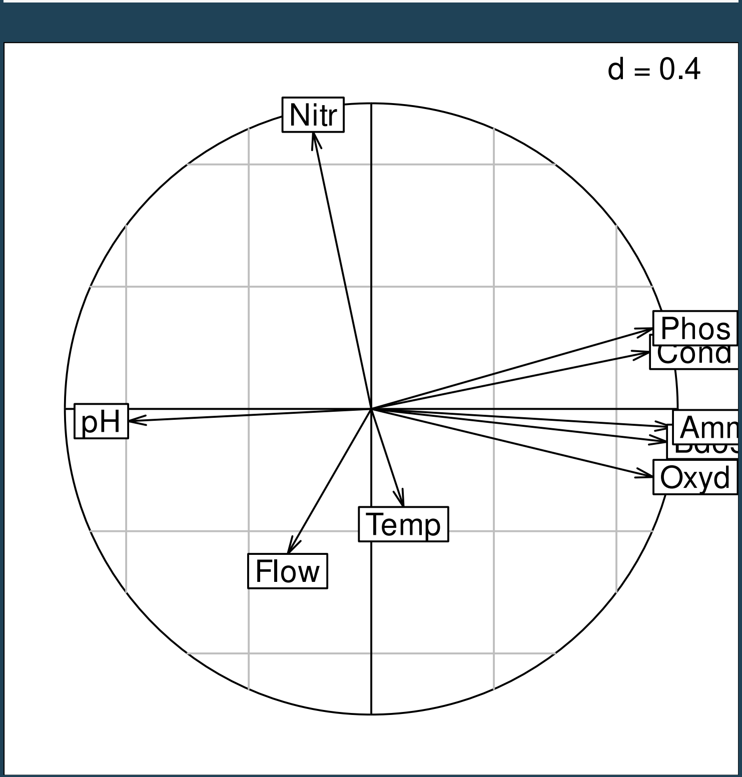


Separate representations

```
s.label(pca.meau$li)
```

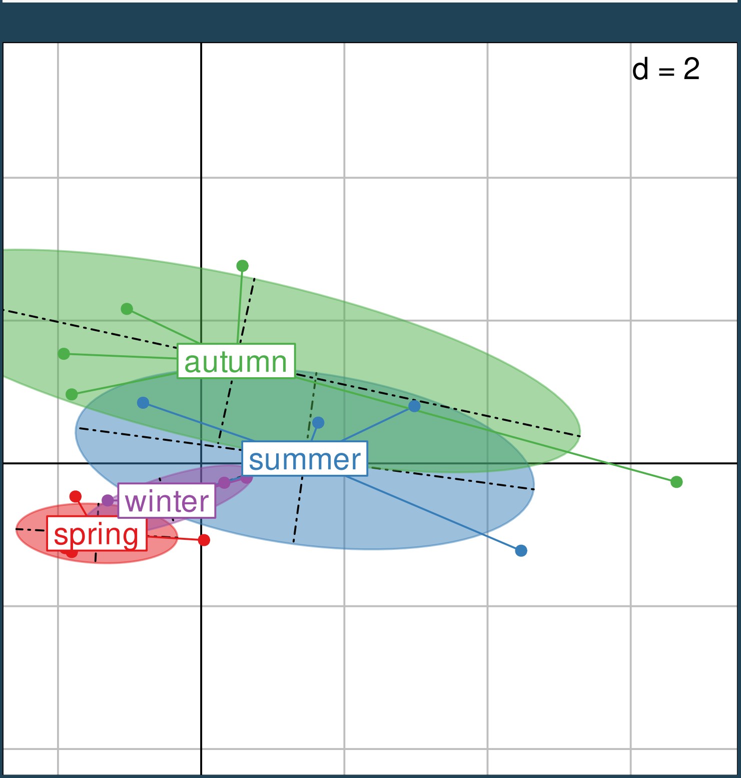


```
s.corcircle(pca.meau$co)
```

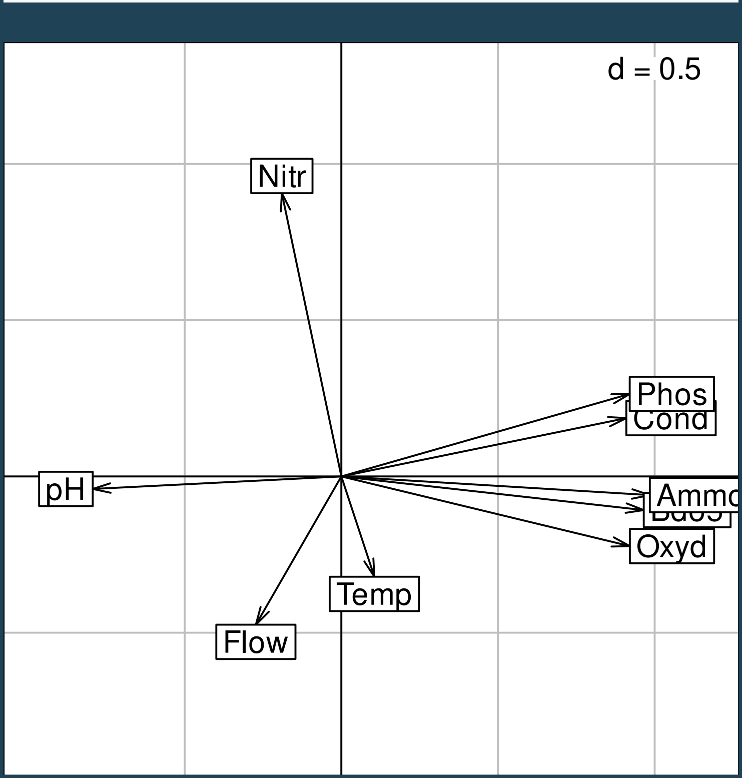


Separate representations

```
s.class(pca.meau$li, meaudret$des
```



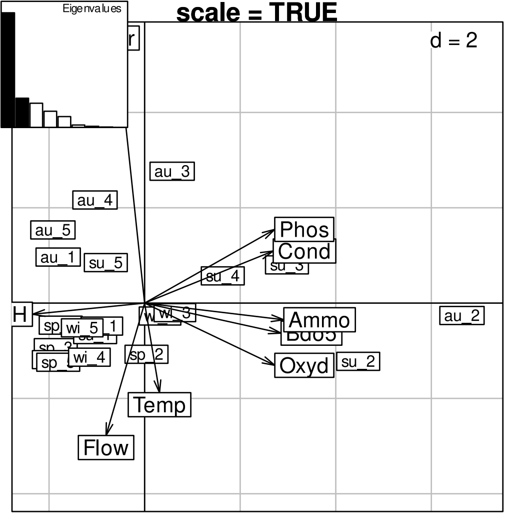
```
s.arrow(pca.meau$co)
```

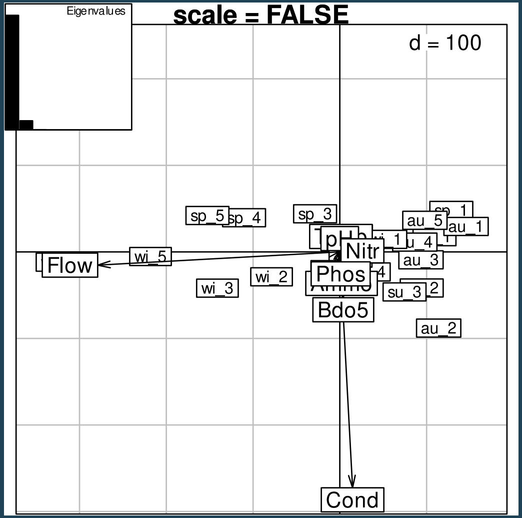


To scale or not to scale

Scaling should be performed when we do not want that differences in variances affect the results

```
pca.meau.c <- dudi.pca(meaudret$env, scannf = FALSE,
    scale = FALSE)
```





In our case, we must scale the data as differences in variances are mainly due to differences in units

Inertia statistics

```
summary(pca.meau)
```

```
## Class: pca dudi
## Call: dudi.pca(df = meaudret$env, scannf = FALSE)
##
## Total inertia: 9
##
## Eigenvalues:
##     Ax1     Ax2     Ax3     Ax4     Ax5
##  5.1747  1.3204  1.0934  0.7321  0.4902
##
## Projected inertia (%):
##     Ax1     Ax2     Ax3     Ax4     Ax5
##  57.497  14.671  12.149   8.135   5.447
##
## Cumulative projected inertia (%):
##     Ax1   Ax1:2   Ax1:3   Ax1:4   Ax1:5
##   57.50   72.17   84.32   92.45   97.90
##
## (Only 5 dimensions (out of 9) are shown)
```

PCA in practice

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