Raw-data and distance based methods

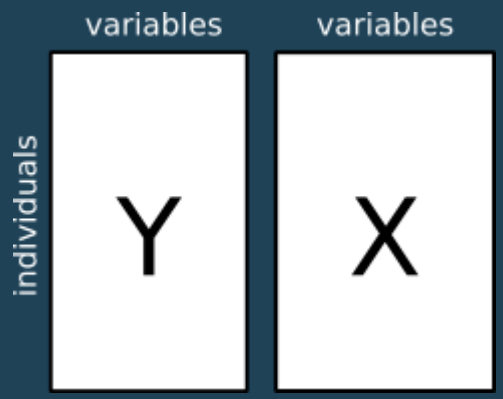
in practice

Stéphane Dray

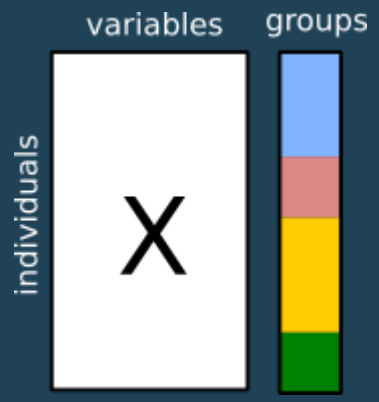
2024-01-08

Raw data

Principal Component Analysis

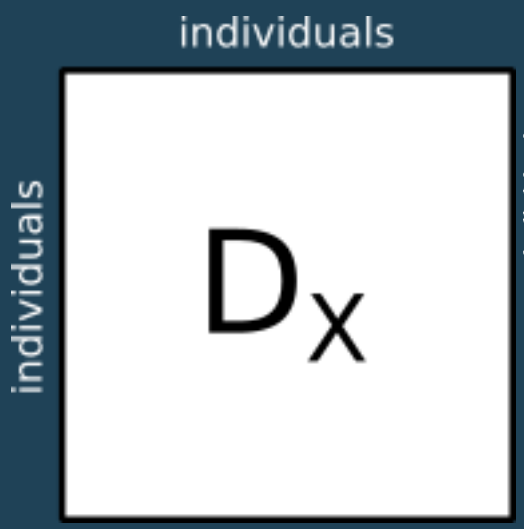


Co-Inertia Analysis

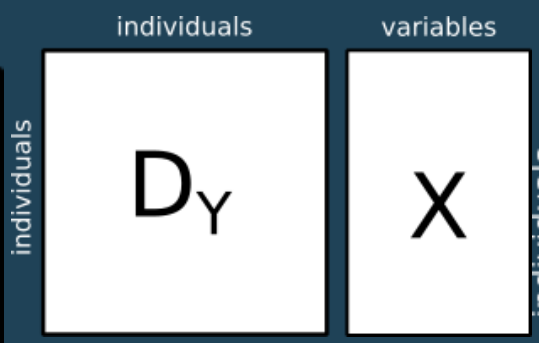


Between-Class Analysis

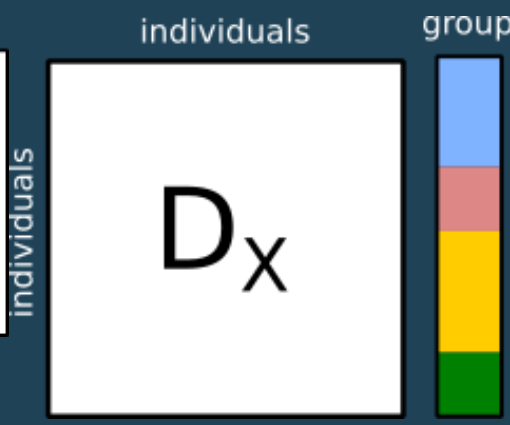
Distances



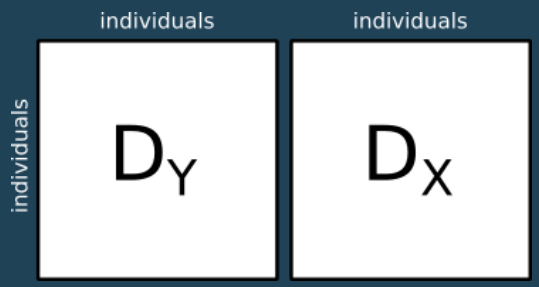
Principal Coordinates Analysis



Distance-Based Redundancy Analysis



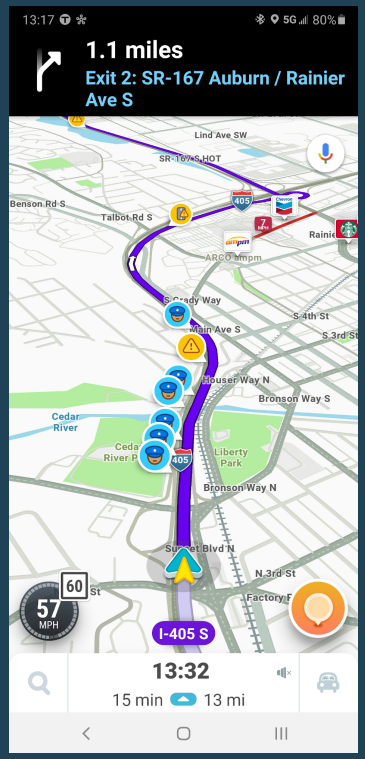
dbRDA, ANOSIM

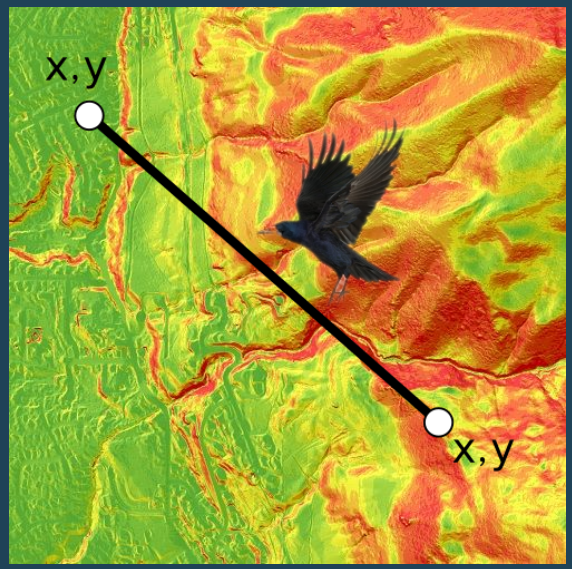


Mantel test

Distance vs Raw

- Distances can be directly measured or inherited from raw-data



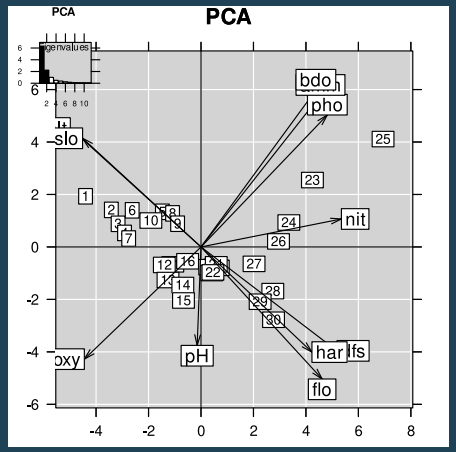


Distance vs Raw

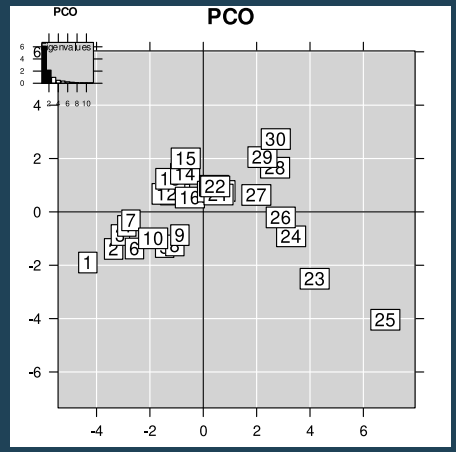
- Raw-data methods produce information on both individuals and variables when distance-based methods focus only on individuals

```
library(ade4)
library(adegraphics)
data(doubs)
pca <- dudi.pca(doubs$env, scannf = FALSE)
pco <- dudi.pco(dist(scale(doubs$env)), scannf = FALSE)
```

```
scatter(pca, main = "PCA")
```




```
scatter(pco, main = "PCO")
```



Distance vs Raw

- Distance-based methods allow for more flexibility and can be more suitable in some contexts

```
x
```

```
##        species 1 species 2 species 3 species 4
## site 1         1         1         0         1
## site 2         0         0         0         1
## site 3         1         1         1         1
## site 4         0         0         1         1
```

```
## Euclidean
round(dist(x), 2)
```

```
##        site 1 site 2 site 3
## site 2   1.41
## site 3   1.00   1.73
## site 4   1.73   1.00   1.41
```

```
## Jaccard
round(dist.binary(x, method = 1),
```

```
##        site 1 site 2 site 3
## site 2   0.82
## site 3   0.50   0.87
## site 4   0.87   0.71   0.71
```

Sites 3-4 are closer than sites 1-2 when considering only presences as a measure of similarity

Distance vs Raw

- In some cases, both approaches can be equivalent (Euclidean distances)

For the univariate case, Euclidean distance is $d_{ij} = \sqrt{(x_i - x_j)^2}$ and we have:

$$var(\mathbf{x}) = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2 = \frac{1}{2n^2}\sum_{i=1}^{n}\sum_{j=1}^{n} d_{ij}^2$$

```
x <- rnorm(10)
var(x) * 9/10
```

```
## [1] 0.8787088
```

```
sum(as.matrix(dist(x))^2)/(2 * 10^2)
```

```
## [1] 0.8787088
```

When using Euclidean distance, several raw- and distance-based analysis would produce the same results.

Your turn

1. Create an Rmd file
2. Load the `meaudret` data set from `ade4`
3. Perform the principal component analysis (`dudi.pca`) and principal coordinates analysis (`dudi.pco`) using Euclidean distances (`dist`) on faunistic data. Compare the outputs and conclude.
4. Transform the data into presence-absence (`ifelse(meaudret$spe>0, 1, 0)`). Peform principal coordinates analysis (`dudi.pco`) using Euclidean (`dist`) and Jaccard distances (`dist.binary`). Compare the results.
5. Perform the between-class analysis (`bca`) and distance-based RDA (`vegan::dbrda`) using Euclidean distances using the factor `meaudret$design$season` as an exploratory variable. Compare the results (be aware that `vegan` use $\frac{1}{n-1}$ to compute variances while `ade4` uses $\frac{1}{n}$).
6. Look at the percentage of variation explained by the between-class analysis (stored in the object). Perform permutational multivariate analysis of variance with the function `vegan::adonis` using the Euclidean distances. Compare

Summary

When using Euclidean distances, we have:

- Principal Coordinates Analysis $\Leftrightarrow$ Principal Component Analysis
- Distance-based Redundancy Analysis $\Leftrightarrow$ Redundancy Analysis (Between-Class Analysis when a single factor is used as explanatory variable)
- Permutational Distance-based Multivariate Analysis of Variance $\Leftrightarrow$ Permutation test of Between-Class Analysis