

Multivariate Lake Data Example

Applied Statistics – A Practical Course

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0.1 Introduction

The following example demonstrates basic multivariate principles by means of a teaching example. A detailed description of theory and applications is found in excellent books of Legendre & Legendre (1998) and Borcard et al. (2018). Practical help is found in the tutorials of the **vegan** package (Oksanen et al., 2020).

0.2 Data set and terms of use

The lake data set originates from the public data repository of the German Umweltbundesamt (Umweltbundesamt, 2021). The data set provided can be used freely according to the [terms and conditions](#) published at the [UBA web site](#), that refer to § 12a EGovG with respect of the data, and to the [Creative Commons CC-BY ND International License 4.0](#) with respect to other objects directly created by UBA.

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0.3 Load the data

Here we load the data set and add English column names and abbreviated lake identifiers as row names to the table, that are useful for the multivariate plotting functions.

```
library("readxl") # read Excel files directly
library("vegan")  # multivariate statistics in ecology
lakes <- as.data.frame(
  read_excel("../data/uba/3_tab_kenndaten-ausgew-seen-d_2021-04-08.xlsx", sheet="Tabelle1")
)
names(lakes) <- c("name", "state", "drainage", "population", "altitude",
                  "z_mean", "z_max", "t_ret", "volume", "area", "shore_length",
                  "shore_devel", "drain_ratio", "wfd_type")
rownames(lakes) <- paste0(1:nrow(lakes), substr(lakes$name, 1, 4))
```

Text columns, e.g Federal State names and lake type are removed and rows with missing data excluded. If population is not used, the analysis can be repeated with more lakes.

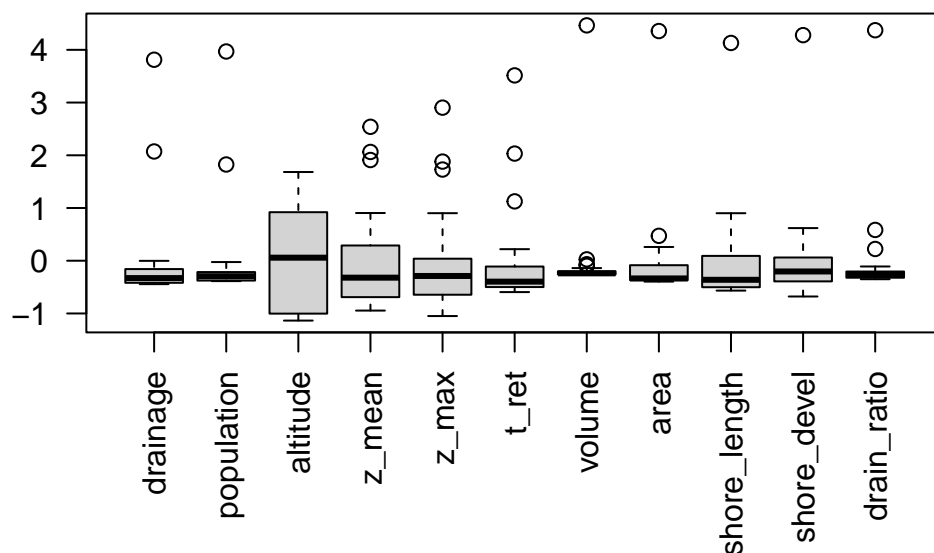
```
valid_columns <- c("drainage", "population", "altitude", "z_mean",  
                  "z_max", "t_ret", "volume", "area", "shore_length",  
                  "shore_devel", "drain_ratio")  
  
#valid_columns <- c("drainage", "altitude", "z_mean",  
#                  "z_max", "t_ret", "volume", "area", "shore_length",  
#                  "shore_devel", "drain_ratio")  
dat <- lakes[valid_columns]  
dat <- na.omit(dat)
```

0.4 Data inspection

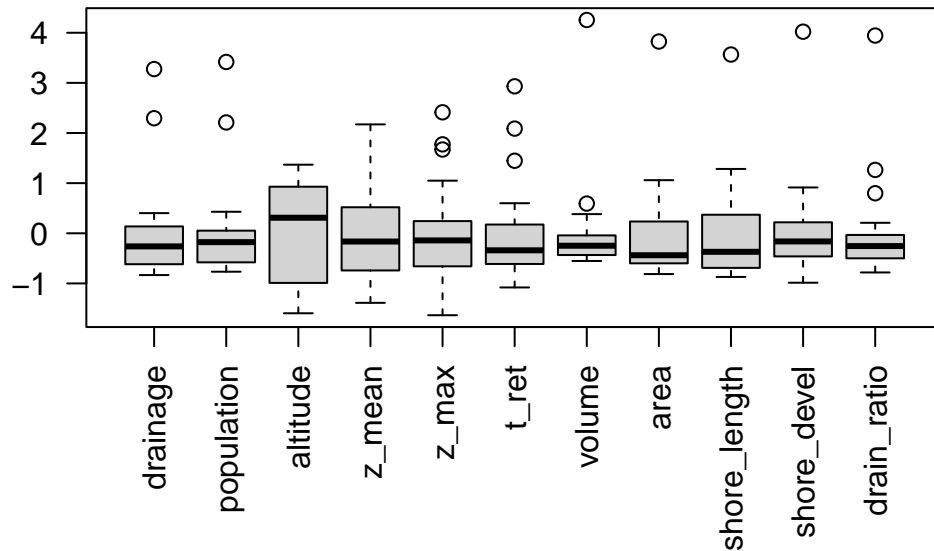
It is always a good idea to plot the data first, as time series or boxplots for example, depending on the type of data. Here we use boxplots, that we scale (z-transform) to a mean zero and standard deviation one to have comparable values.

As we can see a number of high extreme values, we apply also a square root transformation, that is less extreme than log transform and not sensitive against zero values, but because altitude contains a negative value (below sea level) we replace this with zero. As it is a small value, it does not influence our analysis, but we should always be very careful to document such workarounds.

```
par(mfrow = c(1, 1))  
par(mar = c(7, 4, 2, 1) + .1)  
boxplot(scale(dat), las = 2)
```



```
dat$altitude <- ifelse(dat$altitude < 0, 0, dat$altitude)
boxplot(scale(sqrt(dat)), las=2)
```



0.5 Multivariate Analysis

0.5.1 Principal Components: PCA

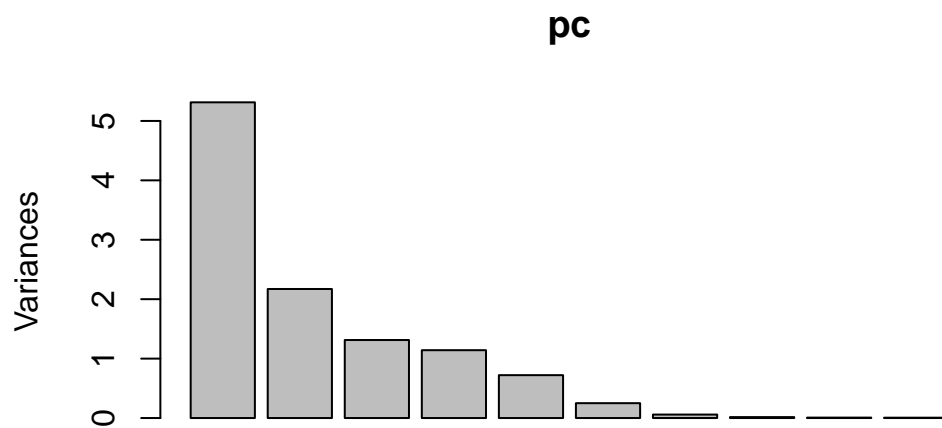
```
pc <- prcomp(scale(dat))
summary(pc)
```

Importance of components:

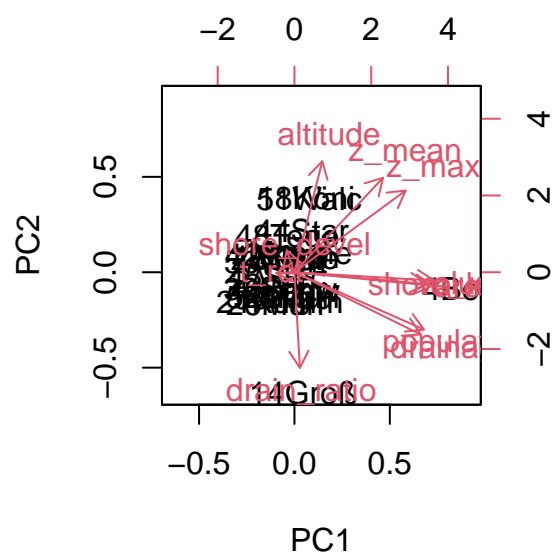
| | PC1 | PC2 | PC3 | PC4 | PC5 | PC6 | PC7 |
|------------------------|-------|--------|--------|--------|---------|---------|---------|
| Standard deviation | 2.305 | 1.4737 | 1.1459 | 1.0686 | 0.84953 | 0.50024 | 0.24164 |
| Proportion of Variance | 0.483 | 0.1974 | 0.1194 | 0.1038 | 0.06561 | 0.02275 | 0.00531 |
| Cumulative Proportion | 0.483 | 0.6805 | 0.7998 | 0.9036 | 0.96925 | 0.99200 | 0.99731 |

| | PC8 | PC9 | PC10 | PC11 |
|------------------------|---------|---------|---------|---------|
| Standard deviation | 0.12590 | 0.08400 | 0.07563 | 0.03077 |
| Proportion of Variance | 0.00144 | 0.00064 | 0.00052 | 0.00009 |
| Cumulative Proportion | 0.99875 | 0.99939 | 0.99991 | 1.00000 |

```
plot(pc)
```



```
biplot(pc)
```



As the PCA with the untransformed data looks somewhat asymmetric, we repeat it with square transformed data. In addition, also the 3rd PC is plotted.

```
dat2 <- sqrt(dat)
pc2 <- prcomp(scale(dat2))
summary(pc2)
```

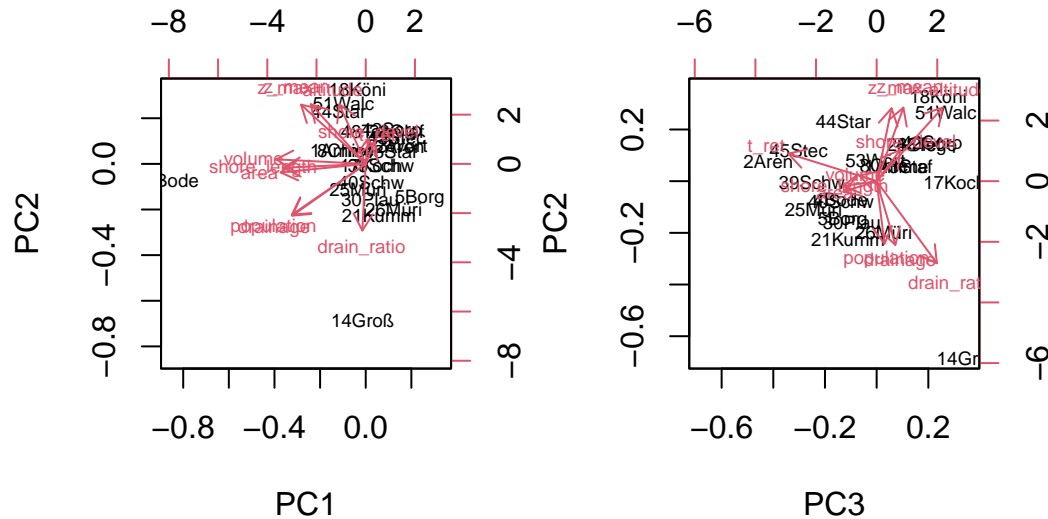
Importance of components:

| | PC1 | PC2 | PC3 | PC4 | PC5 | PC6 | PC7 |
|------------------------|--------|--------|--------|--------|---------|---------|---------|
| Standard deviation | 2.1886 | 1.5906 | 1.2499 | 1.0634 | 0.79782 | 0.44854 | 0.28572 |
| Proportion of Variance | 0.4354 | 0.2300 | 0.1420 | 0.1028 | 0.05786 | 0.01829 | 0.00742 |
| Cumulative Proportion | 0.4354 | 0.6654 | 0.8075 | 0.9103 | 0.96812 | 0.98641 | 0.99383 |

| | PC8 | PC9 | PC10 | PC11 |
|------------------------|---------|---------|---------|---------|
| Standard deviation | 0.17665 | 0.13833 | 0.12041 | 0.05528 |
| Proportion of Variance | 0.00284 | 0.00174 | 0.00132 | 0.00028 |

Cumulative Proportion 0.99666 0.99840 0.99972 1.00000

```
par(mfrow=c(1,2))
par(mar=c(5, 4, 4, 2) + 0.1)
biplot(pc2, cex=0.6)
biplot(pc2, cex=0.6, choices=c(3, 2))
```



A PCA is also possible with the `rda` function of the **vegan** package. The syntax of the plot functions is somewhat different. Instead of `biplot` as above, we can directly use `plot`. Details are found in the **vegan** documentation.

```
par(mfrow=c(1,1))
pc3 <- rda(dat2, scale = TRUE)
plot(pc3)
```

Call: `rda(X = dat2, scale = TRUE)`

-- Model Summary --

| | Inertia | Rank |
|---------------|---------|------|
| Total | 11 | |
| Unconstrained | 11 | 11 |

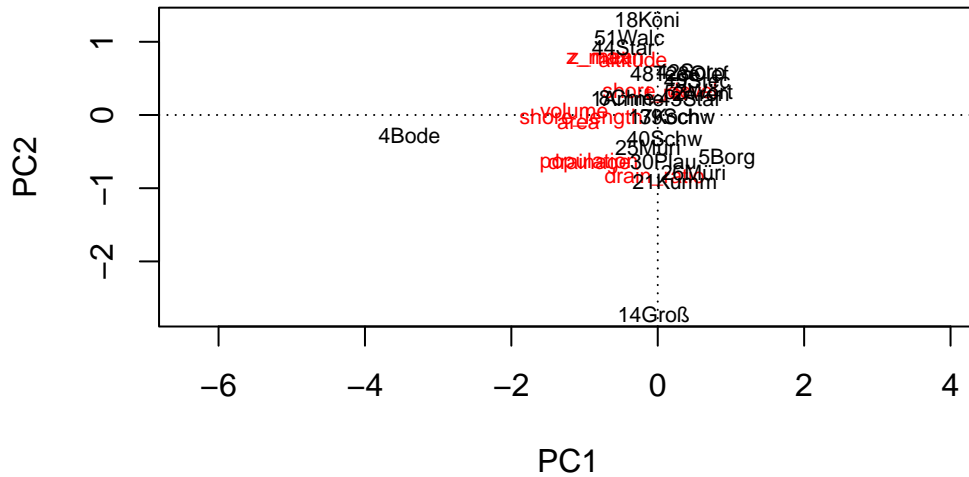
Inertia is correlations

-- Eigenvalues --

Eigenvalues for unconstrained axes:

| PC1 | PC2 | PC3 | PC4 | PC5 | PC6 | PC7 | PC8 | PC9 | PC10 | PC11 |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| 4.790 | 2.530 | 1.562 | 1.131 | 0.637 | 0.201 | 0.082 | 0.031 | 0.019 | 0.014 | 0.003 |

```
#summary(pc3)
plot(pc3)
```



0.5.2 Nonmetric Multidimensional Scaling: NMDS

Let's now perform an NMDS for the data set. Function `metaMDS` runs a series of NMDS fits with different start values to avoid local minima. It has also some automatic transformations built in and works usually with the Bray-Curtis dissimilarity, that is used for plants and animal species abundance data. As we work with physical data here, we set the distance measure to "euclidean".

```
md <- metaMDS(dat2, scale = TRUE, distance = "euclid")
```

```

Square root transformation
Wisconsin double standardization
Run 0 stress 0.1181117
Run 1 stress 0.1181116
... New best solution
... Procrustes: rmse 0.000117949   max resid 0.0003338069
... Similar to previous best
Run 2 stress 0.1207018
Run 3 stress 0.1181117
... Procrustes: rmse 0.0001526929   max resid 0.0004356265
... Similar to previous best
Run 4 stress 0.1208974
Run 5 stress 0.1188532
Run 6 stress 0.1276811
Run 7 stress 0.1188526
Run 8 stress 0.1181117

```

```

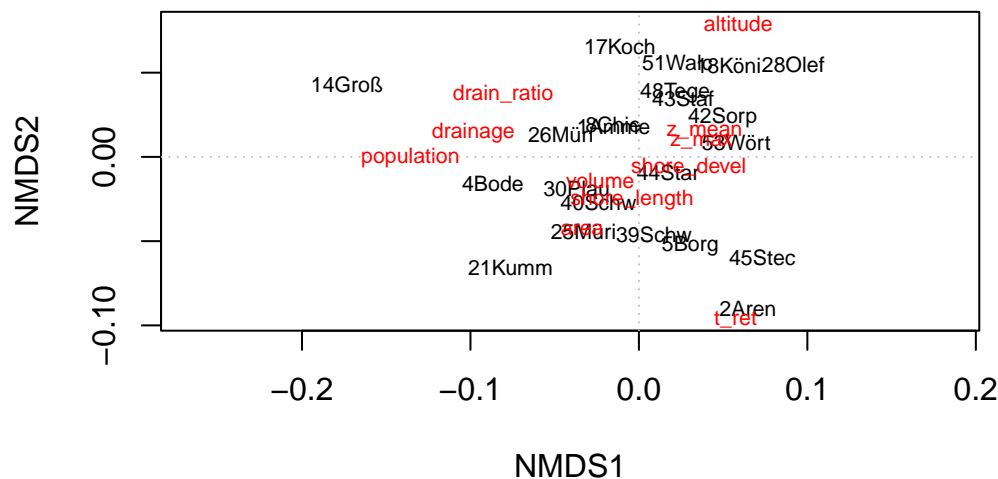
... Procrustes: rmse 0.0001791823  max resid 0.0005133998
... Similar to previous best
Run 9 stress 0.120702
Run 10 stress 0.1230331
Run 11 stress 0.1188537
Run 12 stress 0.1230331
Run 13 stress 0.1181116
... New best solution
... Procrustes: rmse 3.860451e-05  max resid 0.0001222799
... Similar to previous best
Run 14 stress 0.1207019
Run 15 stress 0.1181117
... Procrustes: rmse 0.0001541716  max resid 0.0004881814
... Similar to previous best
Run 16 stress 0.1188268
Run 17 stress 0.1230331
Run 18 stress 0.1207022
Run 19 stress 0.1230331
Run 20 stress 0.1188525
*** Best solution repeated 2 times

```

```

plot(md, type="text")
abline(h=0, col="grey", lty="dotted")
abline(v=0, col="grey", lty="dotted")

```



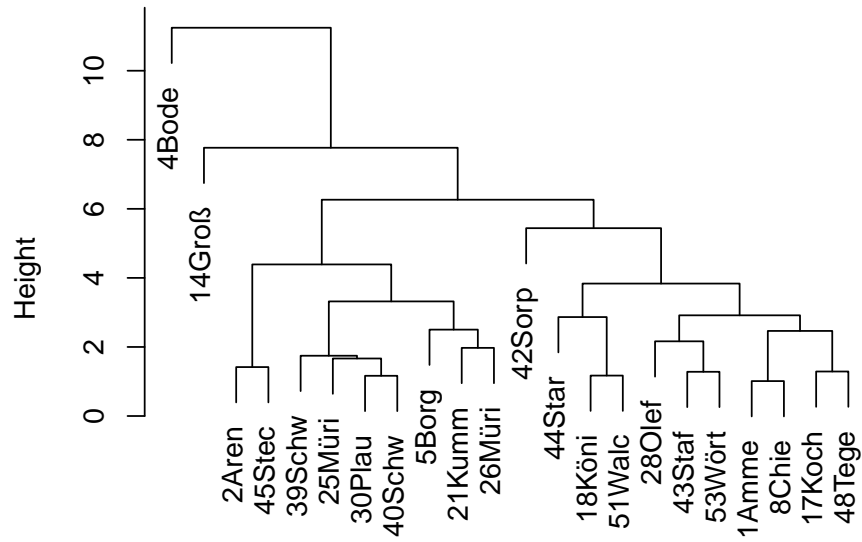
0.5.3 Cluster analysis

Here we apply a hierarchical cluster analysis with square root transformed data and two different agglomeration schemes, “complete linkage” and “Ward’s method”.

```
par(mfrow=c(2,1))
hc <- hclust(dist(scale(dat2)), method="complete") # the default
plot(hc)

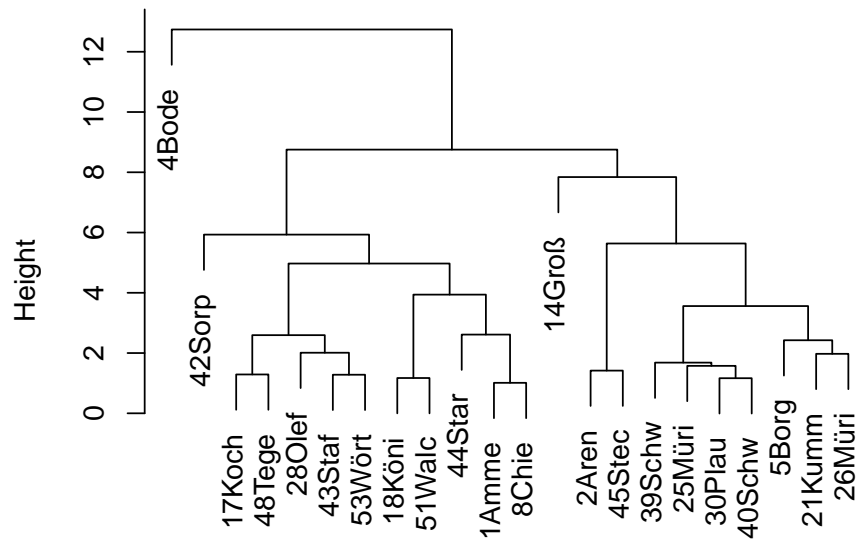
hc2 <- hclust(dist(scale(dat2)), method="ward.D2")
plot(hc2)
```


Cluster Dendrogram



```
dist(scale(dat2))
hclust (*, "complete")
```

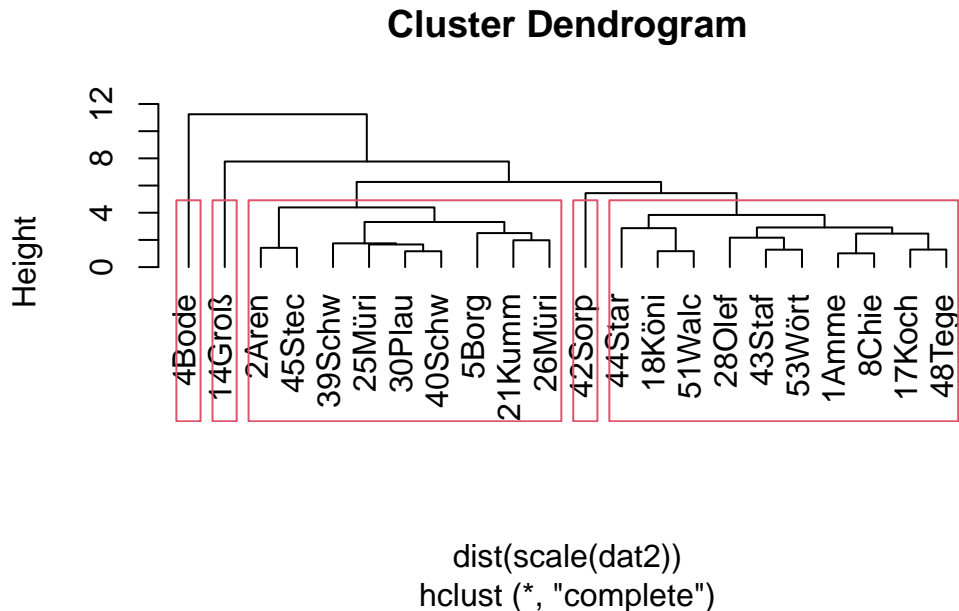
Cluster Dendrogram



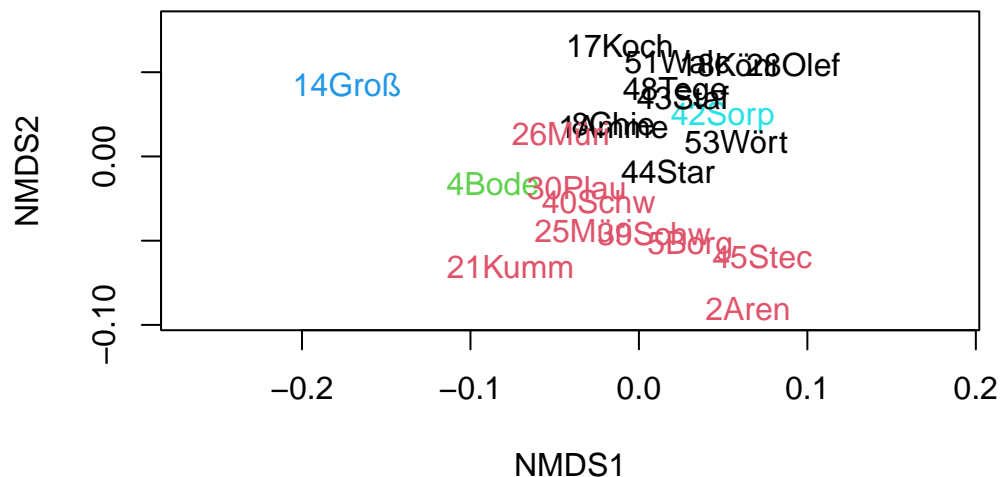
```
dist(scale(dat2))
hclust (*, "ward.D2")
```

We can also use the clusters to indicate groups in the NMDS plot. Function `rect.hclust` indicates a given number of clusters in the dendrogram, then we cut the tree with `cutree` and use the groups `grp` as color codes. **R** has 8 standard colors. If we need more, we can define an own palette.

```
plot(hc, hang = -1)
rect.hclust(hc, 5)
```



```
grp <- cutree(hc, 5)
# grp # can be used to show the groups
plot(md, type = "n")
text(md$points, row.names(dat2), col = grp)
```



Instead of hierarchical clustering, we can also use a non-hierarchical method, e.g. k-means clustering. This is an iterative method, and avoids the problem that cluster assignment depends on the order of clustering and the agglomeration method.

Depending on the question, it may be a disadvantage, that the number of clusters needs to be specified beforehand (e.g. from hierarchical clustering) and that we do not get a tree diagramm.

0.6 Task

- Try to understand the analysis,
- discuss the results,
- ask questions.
- The idea is to work on this report together and to make it more complete.

References

- Borcard, D., Gillet, F., & Legendre, P. (2018). *Numerical Ecology with R*. Springer International Publishing. <https://doi.org/10.1007/978-3-319-71404-2>
- Legendre, P., & Legendre, L. (1998). *Numerical Ecology* (2nd English ed.). Elsevier.
- Oksanen, J., Blanchet, F. G., Friendly, M., Kindt, R., Legendre, P., McGlinn, D., Minchin, P. R., O'Hara, R. B., Simpson, G. L., Solymos, P., Stevens, M. H. H., Szoecs, E., & Wagner, H. (2020). *Vegan: Community ecology package*. <https://CRAN.R-project.org/package=vegan>
- Umweltbundesamt. (2021). *Kenndaten ausgewählter Seen Deutschlands*. <https://www.umweltbundesamt.de/daten/wasser/zustand-der-seen#okologischer-zustand-der-seen>