Solution: Multivariate Lake Data Example

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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.

0.2.1 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("3_tab_kenndaten-ausgew-seen-d_2021-04-08.xlsx", sheet="Tabelle1", skip=3)
)
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.

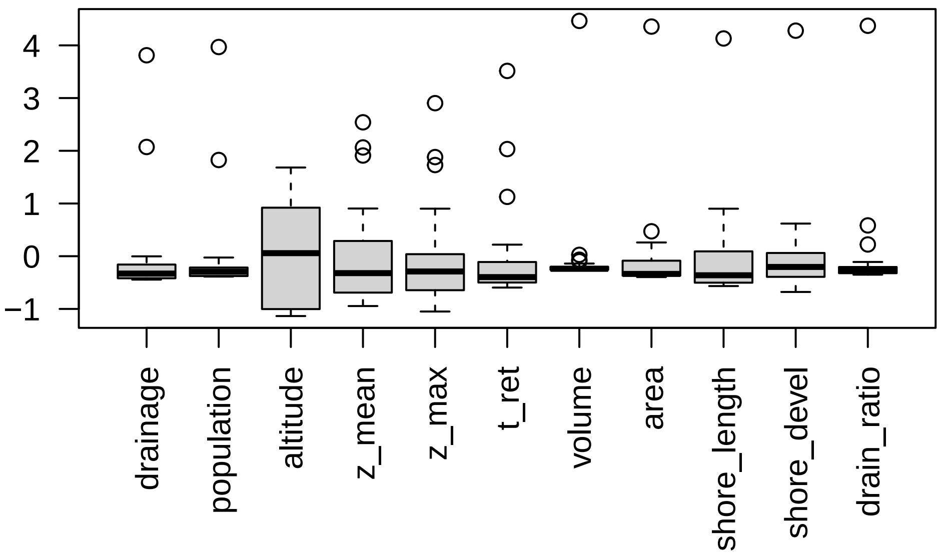
```
valid_columns <- c("drainage", "population", "altitude", "z_mean",
                   "z_max", "t_ret", "volume", "area", "shore_length",
                   "shore_devel", "drain_ratio")

#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)
```

0.2.2 Data inspection

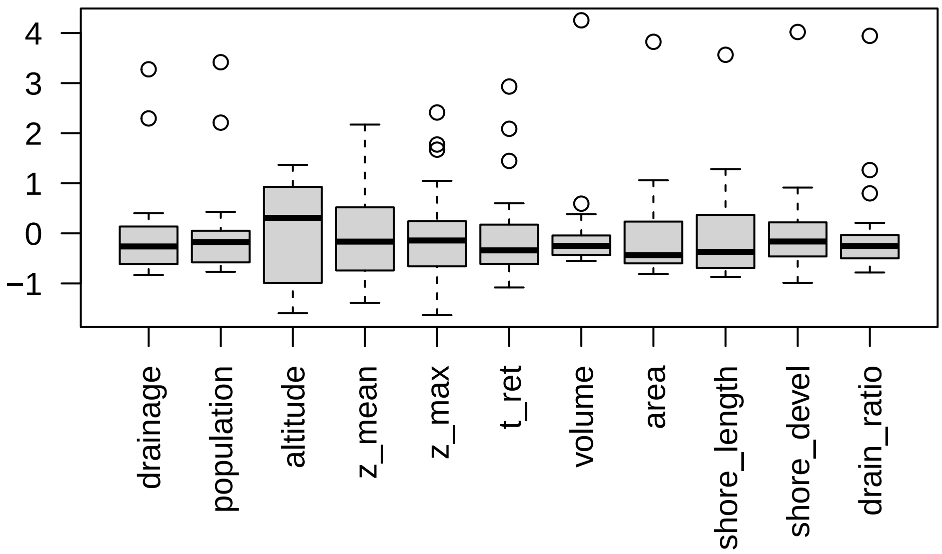
It is always a good idea to plot the data first, either as a time series or as boxplots, depending on the type of data. Here, we use boxplots that we scale (z-transform) to a mean of zero and a standard deviation of one, in order to make the values comparable.

As there are a number of extreme values, we also apply a square root transformation, which is less extreme than a log transformation and not sensitive to zero values. However, as altitude contains a negative value (below sea level), we replace this with zero. As this is a small value, it does not influence our analysis, but we should always document such workarounds carefully.

```
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)
```



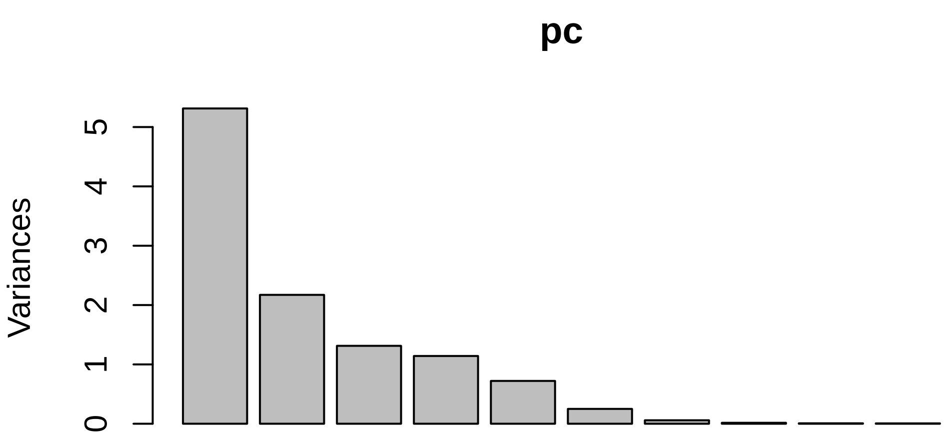
0.3 Multivariate Analysis

0.3.1 Principal Components: PCA

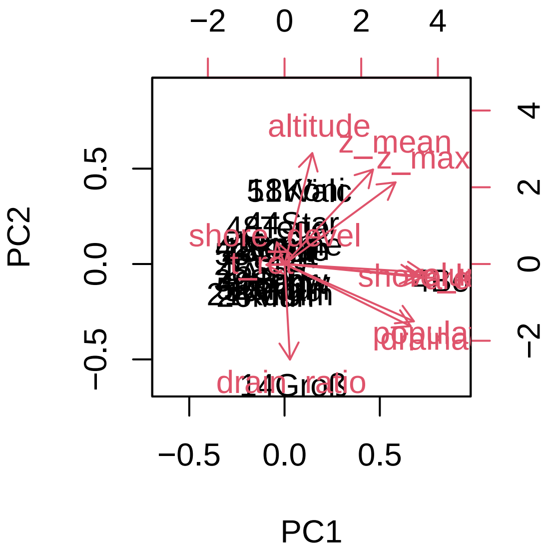
```
pc <- prcomp(scale(dat))
summary(pc)
```

```
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)
```

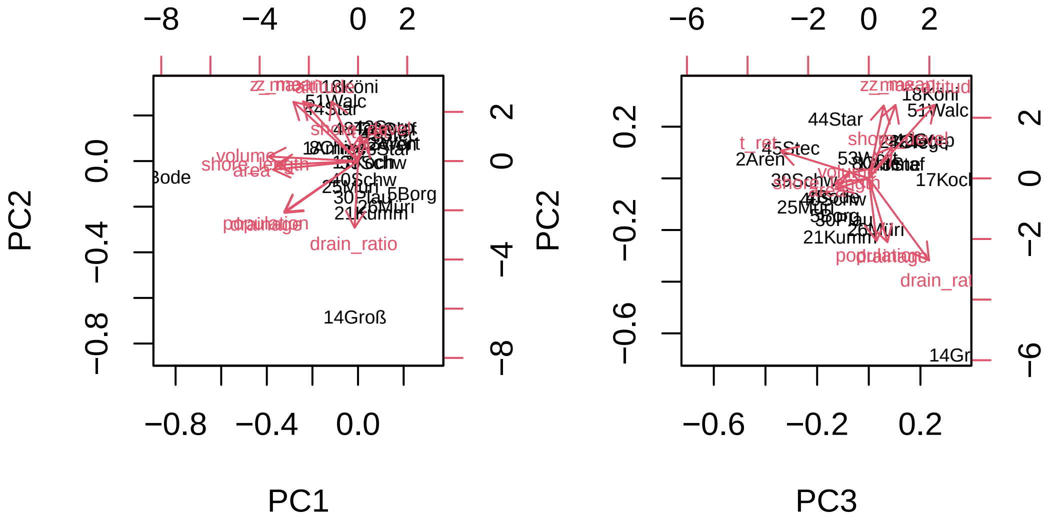


As the PCA with the untransformed data appears somewhat asymmetric, we repeat the process with square-transformed data. Additionally, the third PC is plotted.

```
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))
```

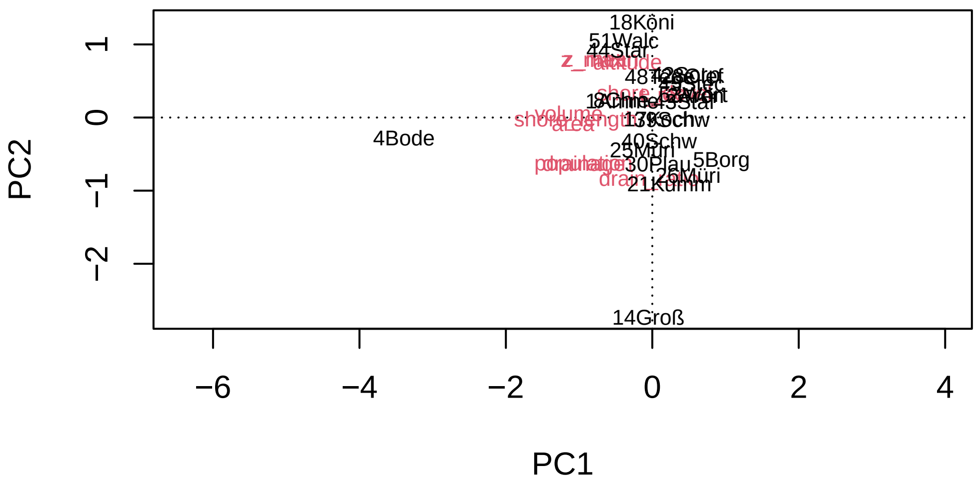


It is also possible to perform a PCA using the **rda** function of the **vegan** package. The syntax of the plot functions differs somewhat. Rather than using **biplot** as above, we can use **plot** directly. Further details can be found in the **vegan** documentation.

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

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

              Inertia Rank
Total              11
Unconstrained      11   11

Inertia is correlations

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)
```



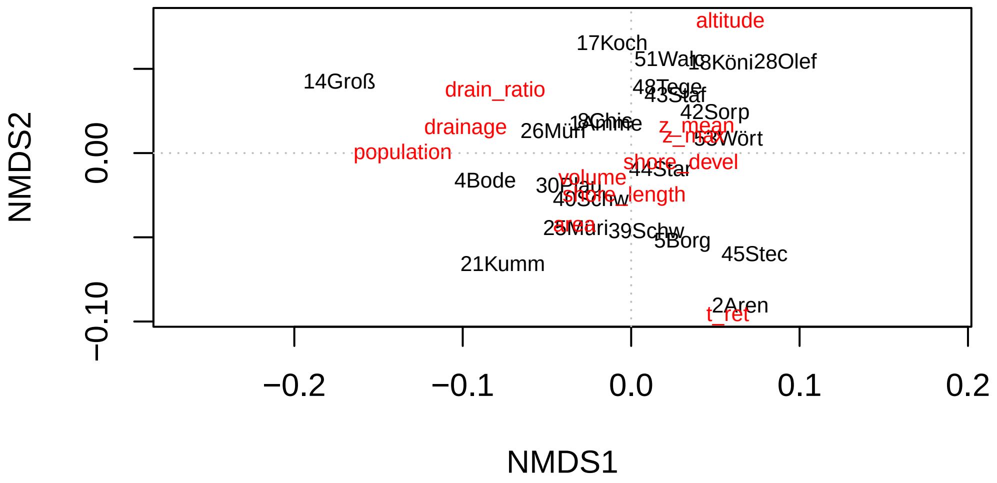
0.3.2 Nonmetric Multidimensional Scaling: NMDS

Now, let's perform an NMDS on the data set. The function `metaMDS` runs a series of NMDS fits with different start values to avoid local minima. It also performs some automatic transformations and usually works with the Bray–Curtis dissimilarity, which is common for plant and animal species abundance data. As we are working with physical data here, we will 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 0.1207019
Run 2 stress 0.1230331
Run 3 stress 0.1768603
Run 4 stress 0.1181117
... New best solution
... Procrustes: rmse 0.000176533  max resid 0.0004978482
... Similar to previous best
Run 5 stress 0.1181118
... Procrustes: rmse 0.0002909119  max resid 0.0008348807
... Similar to previous best
Run 6 stress 0.1230331
Run 7 stress 0.1181116
... New best solution
... Procrustes: rmse 2.095206e-05  max resid 6.60503e-05
... Similar to previous best
Run 8 stress 0.1768603
Run 9 stress 0.1207018
Run 10 stress 0.120702
Run 11 stress 0.1230331
Run 12 stress 0.1207022
Run 13 stress 0.1230331
Run 14 stress 0.1181117
... Procrustes: rmse 8.835998e-05  max resid 0.0003062521
... Similar to previous best
Run 15 stress 0.1208974
Run 16 stress 0.1230331
Run 17 stress 0.1230331
Run 18 stress 0.1230331
Run 19 stress 0.1731461
Run 20 stress 0.1768603
*** Best solution repeated 2 times
```

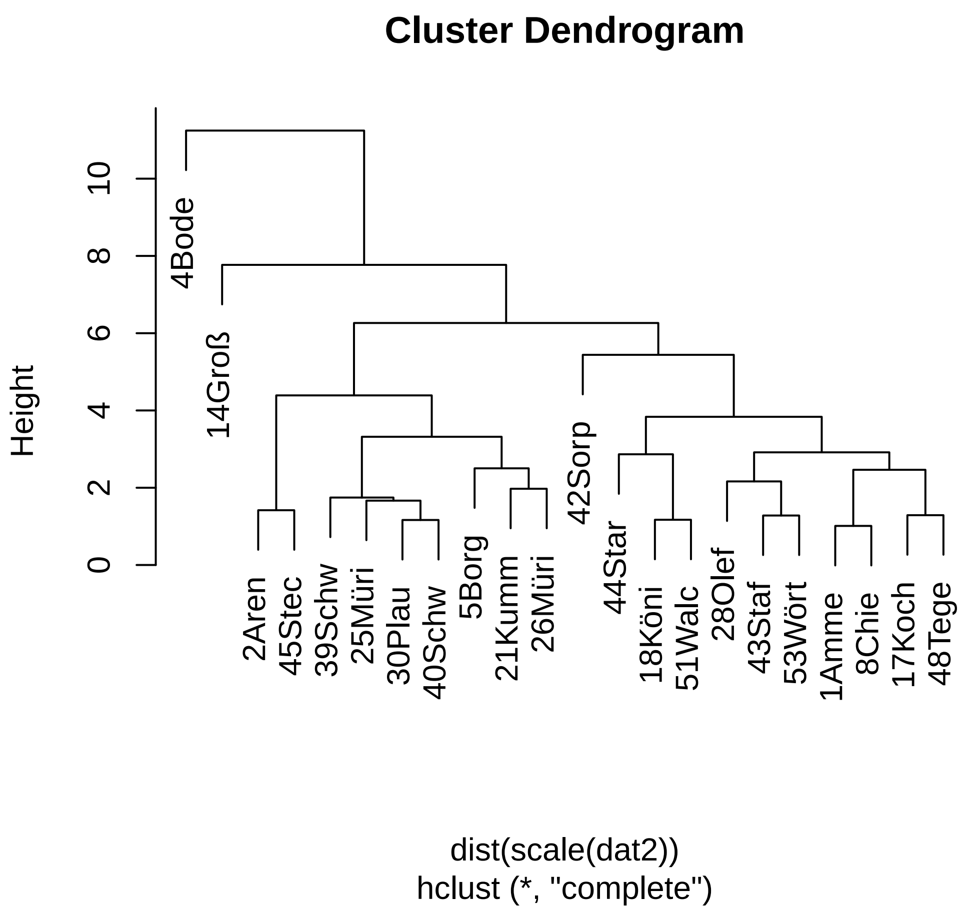
```
plot(md, type="text")
abline(h=0, col="grey", lty="dotted")
abline(v=0, col="grey", lty="dotted")
```

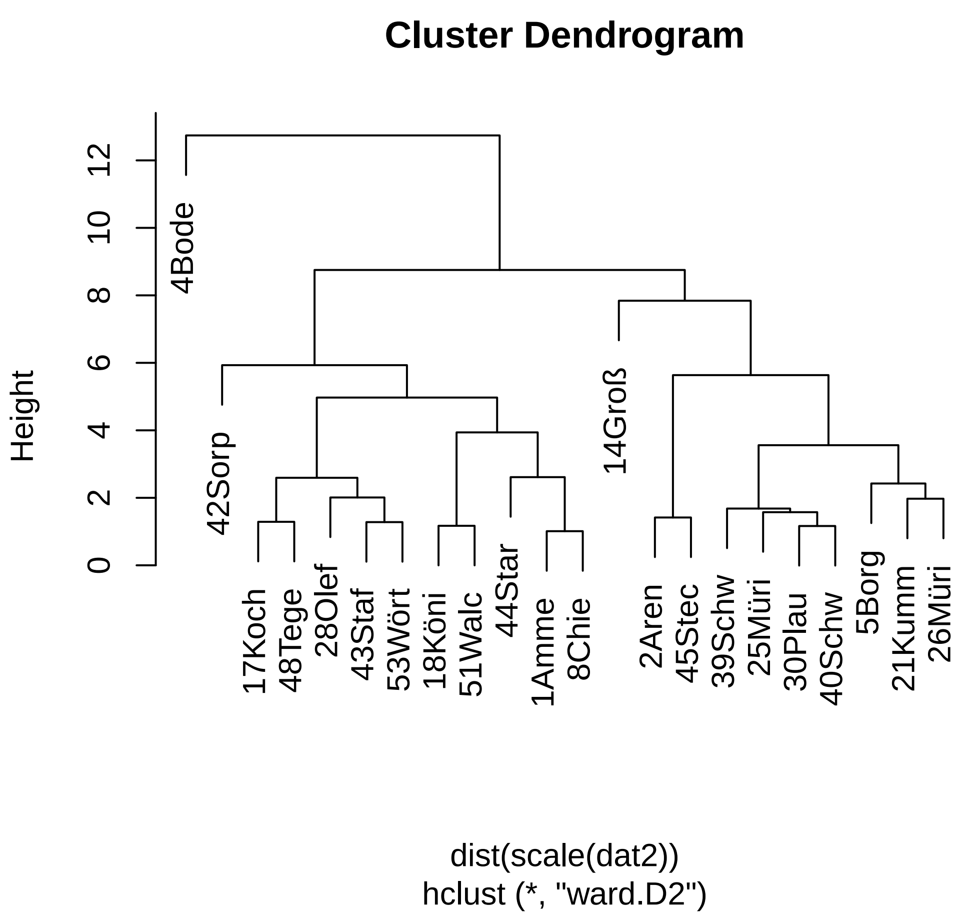


0.3.3 Cluster analysis

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

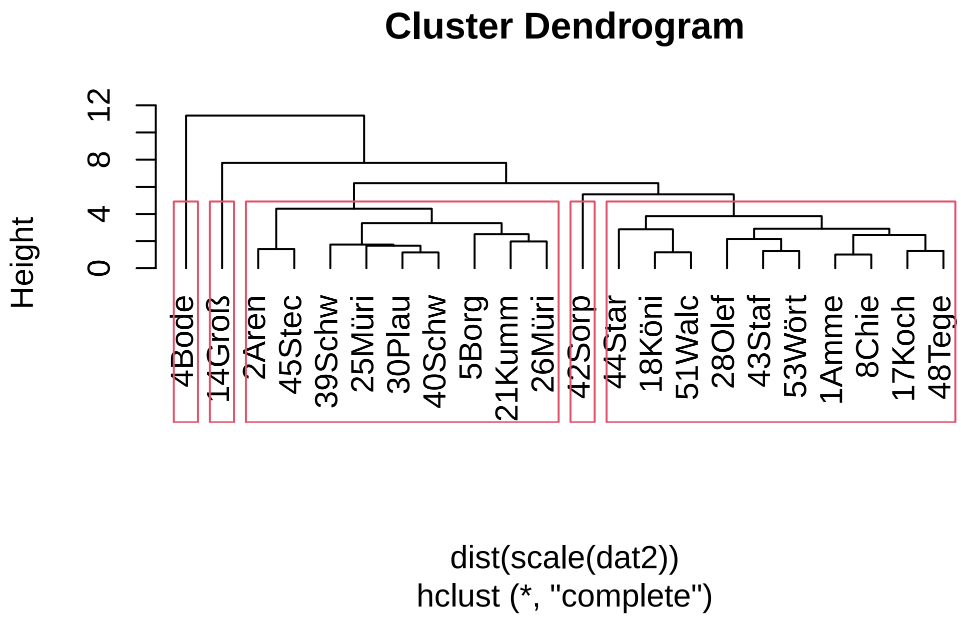
```
par(mfrow=c(2,1))
hc <- hclust(dist(scale(dat2)), method="complete") # the default
plot(hc)

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


Cluster Dendrogram
Height
0
2
4
6
8
10
4Bode
14Groß
42Sorp
2Aren
45Stec
39Schw
25Müri
30Plau
40Schw
5Borg
21Kumm
26Müri
44Star
18Köni
51Walc
28Olef
43Staf
53Wört
1Amme
8Chie
17Koch
48Tege
dist(scale(dat2))
hclust (*, "complete")

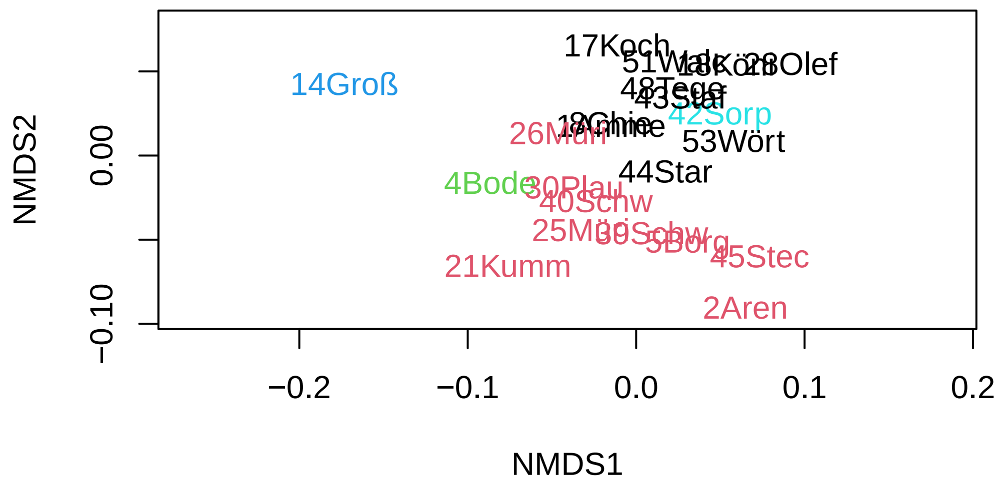

Cluster Dendrogram
Height
0
2
4
6
8
10
12
4Bode
42Sorp
14Groß
17Koch
48Tege
28Olef
43Staf
53Wört
18Köni
51Walc
44Star
1Amme
8Chie
2Aren
45Stec
39Schw
25Müri
30Plau
40Schw
5Borg
21Kumm
26Müri
dist(scale(dat2))
hclust (*, "ward.D2")

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.

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