Multitrait Analysis

I Data preparation

Packages loading

```
library("mclust")
library("Rtsne")
library("ggplot2")
library("reshape2")
library("dplyr")
library("dendextend")
library("cluster")
library("fpc")
library("FactoMineR")
library("factoextra")
```

Data loading

```
df1<-read.csv("trait.tsv", sep ="\t") # omit sep ="\t" for .csv files
```

Clustering continous data

```
df1<-na.omit(df1)
```

```
df1<-df1 %>% arrange(bino)
```

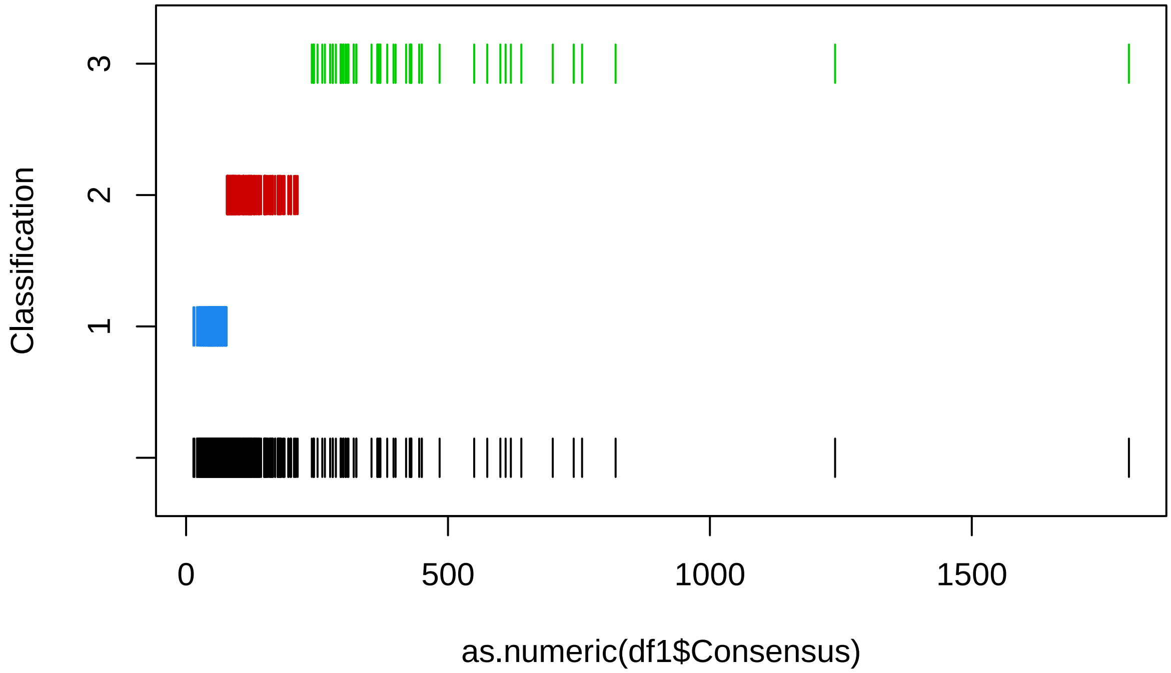
```
mb1 = Mclust(as.numeric(df1$Consensus))
```

```
## fitting ...
##   |                                                                               |
```

```
summary(mb1, parameters = TRUE)
```

```
## ----------------------------------------------------
## Gaussian finite mixture model fitted by EM algorithm
## ----------------------------------------------------
##
## Mclust V (univariate, unequal variance) model with 3 components:
##
##  log-likelihood   n df       BIC       ICL
##       -2970.748 528  8 -5991.65 -6199.418
##
## Clustering table:
##   1   2   3
## 230 241  57
##
## Mixing probabilities:
##         1         2         3
## 0.3757443 0.4886236 0.1356321
##
## Means:
##         1         2         3
##  53.96024 110.22617 371.97834
##
## Variances:
##          1          2          3
##   306.8583  1623.2205 67828.3930
```

```
plot(mb1, what=c("classification")) # plot the discretization
```



```
df1<-(as.data.frame(unclass(df1),stringsAsFactors=TRUE))
```

```
df1$"body_size"<-log(df1$Consensus)
```

```
rownames(df1)<-df1[,1]
df1<-df1[-c(1,2)]
```

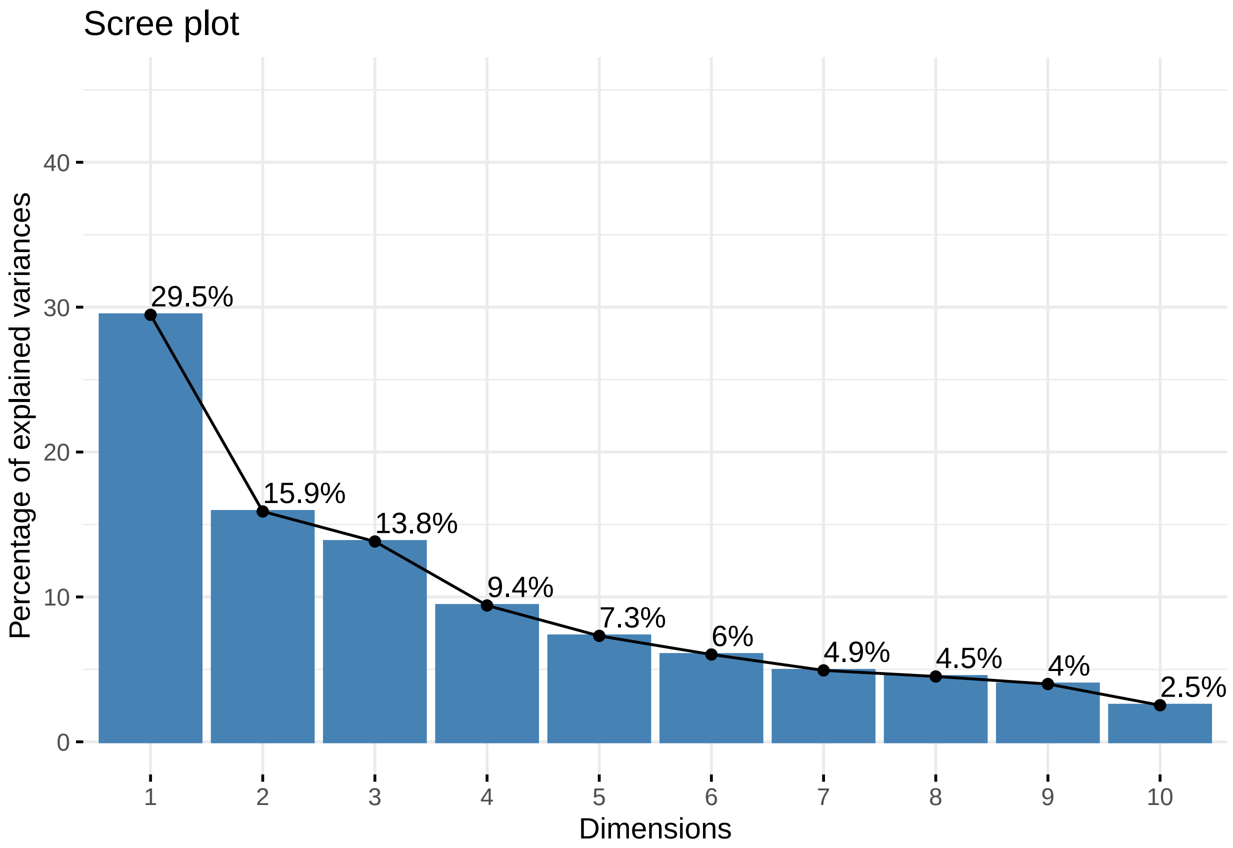
```
df1.1.1<-df1
```

```
df1.1.1$"body_size"<-as.factor(mb1$classification)
```

```
res.mca<-MCA(df1.1.1, ncp = 5, graph = TRUE)
```

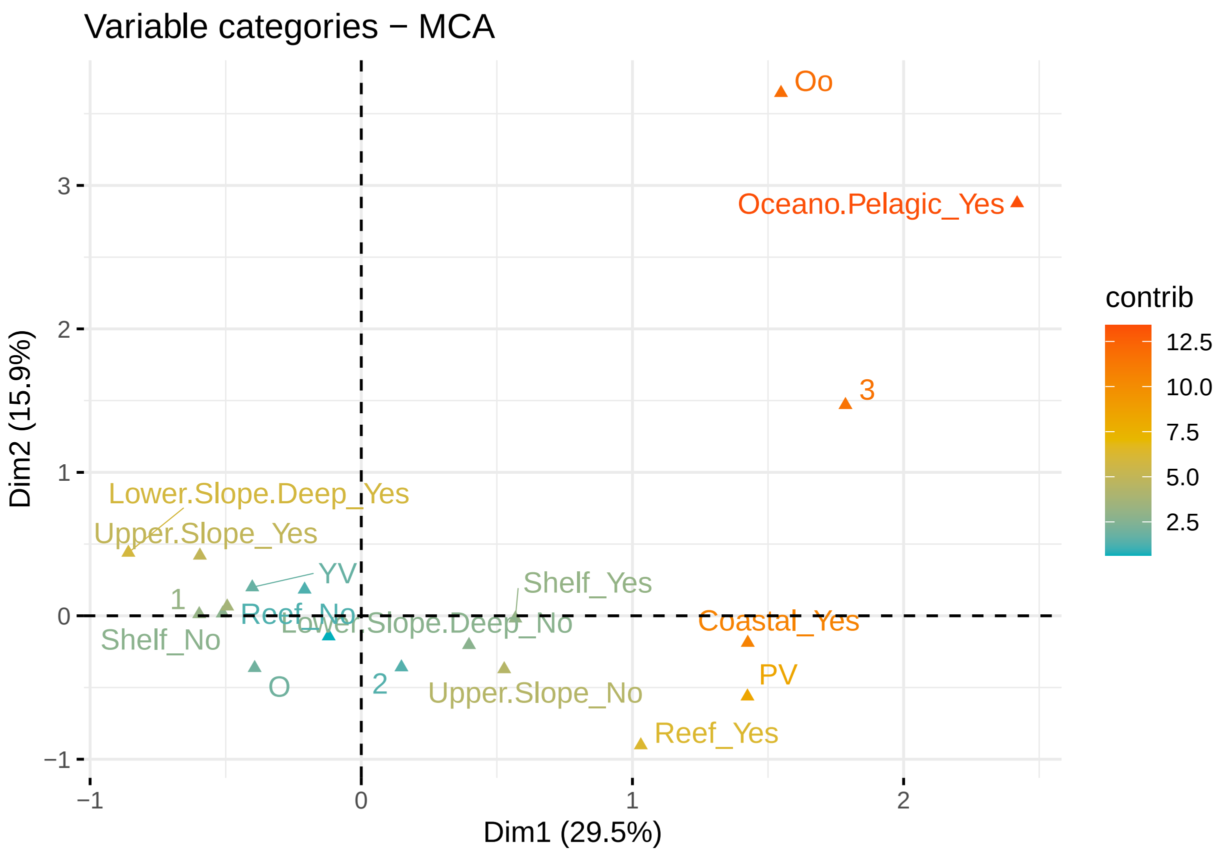
```
eig.val <- get_eigenvalue(res.mca)
```

```
fviz_screeplot(res.mca, addlabels = TRUE, ylim = c(0, 45))
```

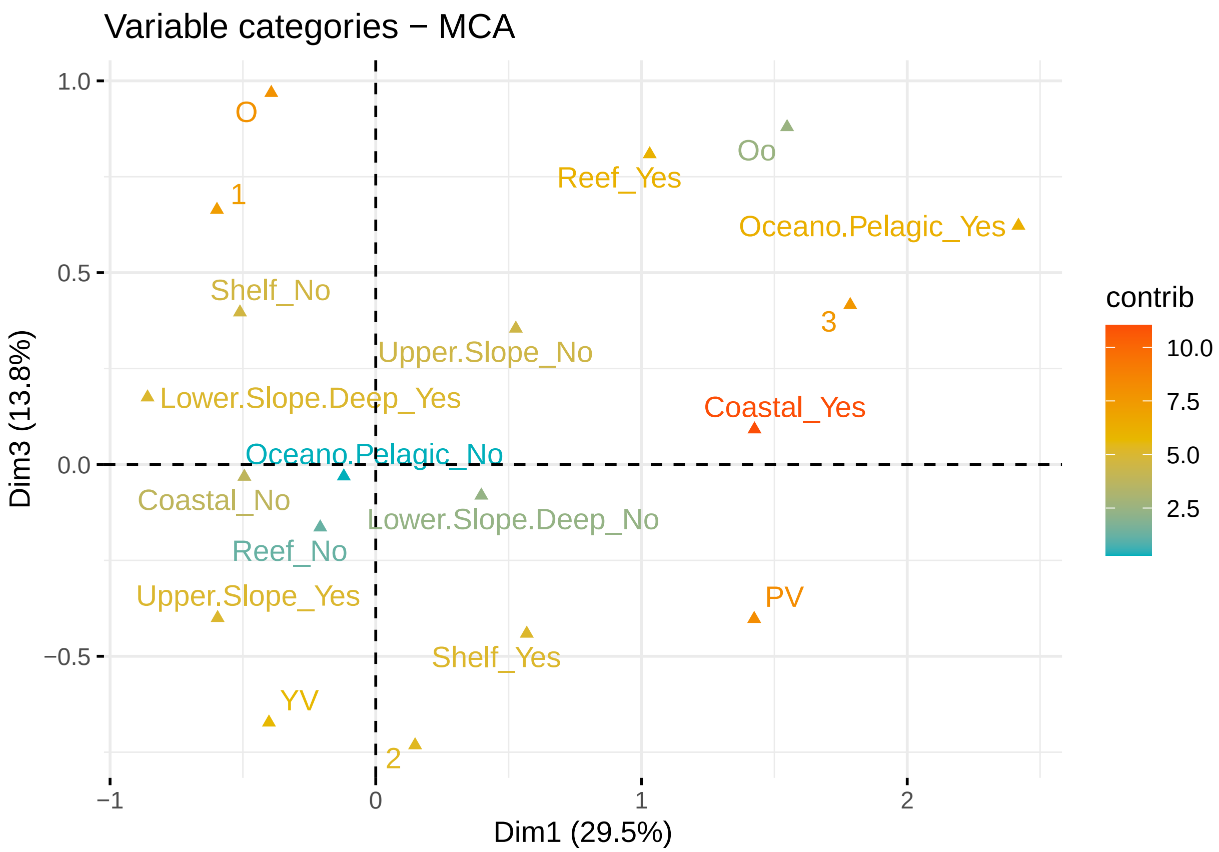


```
fviz_mca_var(res.mca, col.var = "contrib",
             gradient.cols = c("#00AFBB", "#E7B800", "#FC4E07"),
             repel = TRUE, # avoid text overlapping (slow)
             ggtheme = theme_minimal()
             )
```

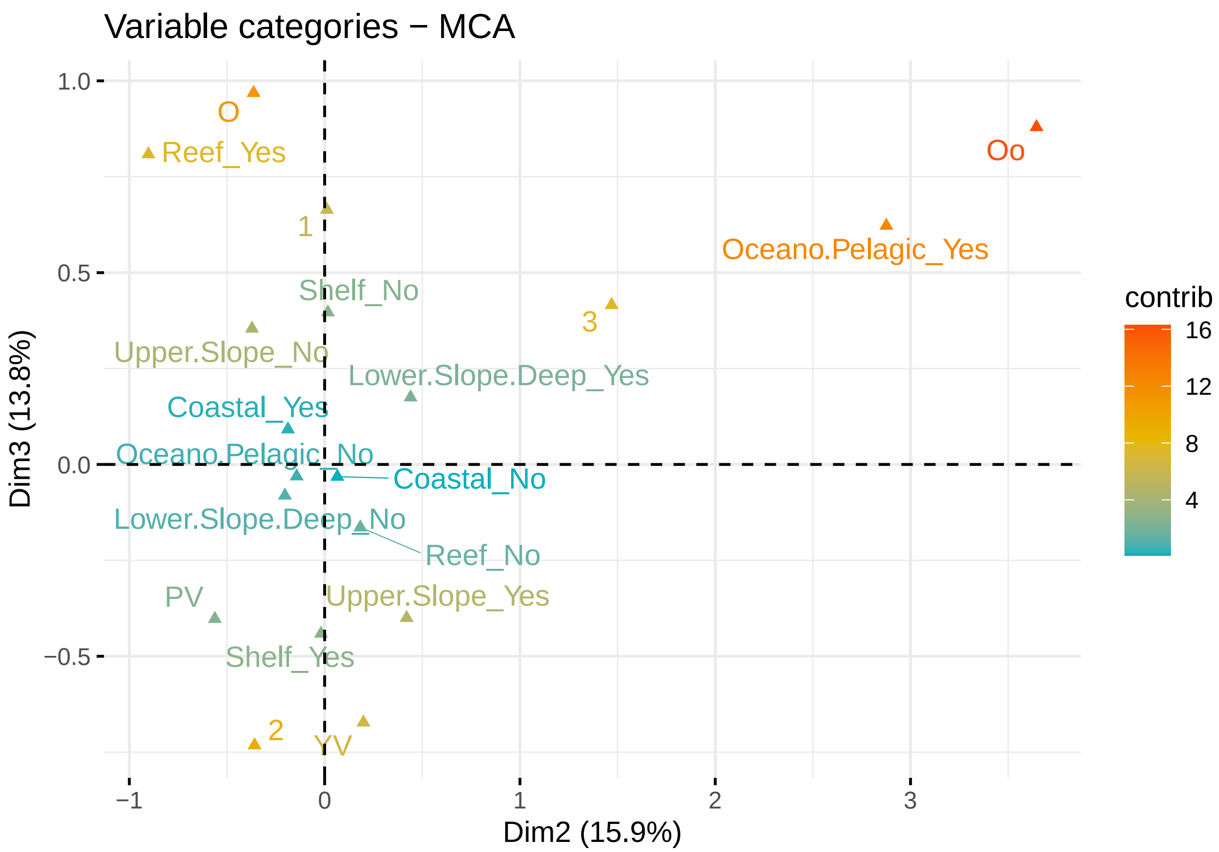
```
## Warning: ggrepel: 2 unlabeled data points (too many overlaps). Consider
## increasing max.overlaps
```



```r
fviz_mca_var(res.mca, axes = c(1,3), col.var = "contrib",
             gradient.cols = c("#00AFBB", "#E7B800", "#FC4E07"),
             repel = TRUE, # avoid text overlapping (slow)
             ggtheme = theme_minimal()
             )
```



```
fviz_mca_var(res.mca, axes = c(2,3), col.var = "contrib",
             gradient.cols = c("#00AFBB", "#E7B800", "#FC4E07"),
             repel = TRUE, # avoid text overlapping (slow)
             ggtheme = theme_minimal()
             )
```



II Hierarchical clustering

Dissimilarity matrix creation

```
gower.dist <- daisy(as.data.frame(df1), metric = c("gower"))
```

```
divisive.clust <- diana(as.matrix(gower.dist),diss = TRUE, keep.diss = TRUE)
aggl.clust.c <- hclust(gower.dist, method = "complete")
aggl.clust.m <- hclust(gower.dist, method = "average")
aggl.clust.w <- hclust(gower.dist, method = "ward.D2")
```

2-norm and least square criterion

Complete

```
sigma <- var(gower.dist)+var(cophenetic(aggl.clust.c))
thres <- 2*sqrt(nrow(as.matrix(gower.dist))*sigma)
sign<-(thres > max(abs(svd(gower.dist-cophenetic(aggl.clust.c))$d)))
col.c<-c("Complete", thres, sign, sum((gower.dist-cophenetic(aggl.clust.c))**2))
```

UPGMA

```
sigma <- var(gower.dist)+var(cophenetic(aggl.clust.m))
thres <- 2*sqrt(nrow(as.matrix(gower.dist))*sigma)
sign<-(thres > max(abs(svd(gower.dist-cophenetic(aggl.clust.m))$d)))
col.m<-c("UPGMA", thres, sign, sum((gower.dist-cophenetic(aggl.clust.m))**2))
```

Ward

```
sigma <- var(gower.dist)+var(cophenetic(aggl.clust.w))
thres <- 2*sqrt(nrow(as.matrix(gower.dist))*sigma)
sign<-(thres > max(abs(svd(gower.dist-cophenetic(aggl.clust.w))$d)))
col.w<-c("Ward", thres, sign, sum((gower.dist-cophenetic(aggl.clust.w))**2))
```

Divisive

```
sigma <- var(gower.dist)+var(cophenetic(divisive.clust))
thres <- 2*sqrt(nrow(as.matrix(gower.dist))*sigma)
sign<-(thres > max(abs(svd(gower.dist-cophenetic(divisive.clust))$d)))
col.div<-c("Divisive", thres, sign, sum((gower.dist-cophenetic(divisive.clust))**2))
```

Comparaison of algorithm dataframe

```
algo_sel <- rbind(col.c, col.m, col.w, col.div)
colnames(algo_sel)<-c("Name", "Threshold value", "Significance", "Least square")
```

```
algo_sel
```

```
##         Name       Threshold value    Significance Least square
## col.c   "Complete" "15.8899480966262" "FALSE"      "17868.6790835317"
## col.m   "UPGMA"    "10.9893698329314" "FALSE"      "2112.97328173017"
## col.w   "Ward"     "94.8679286025524" "FALSE"      "2444751.01318133"
## col.div "Divisive" "15.7310253950952" "FALSE"      "18787.7913794627"
```

```
# Select the best algorithm, here : UPGMA
```

Data repartition visualization

```
# Following the method presented by Anastasia Reusova in her blogpost in Towardsdatascience
```

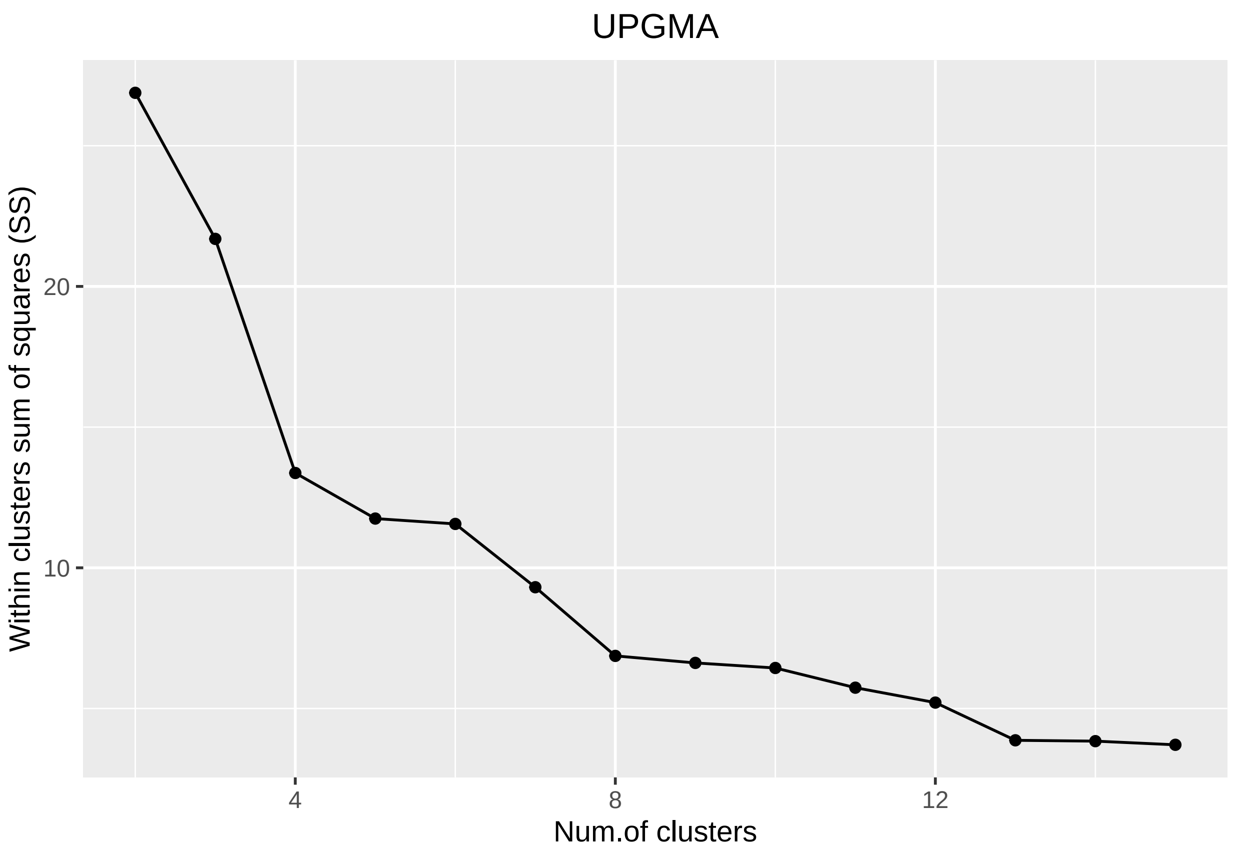
```
cstats.table <- function(dist, tree, k) {
clust.assess <- c("cluster.number","n","within.cluster.ss","average.within","average.between",
                  "wb.ratio","dunn2","avg.silwidth")
clust.size <- c("cluster.size")
stats.names <- c()
row.clust <- c()
output.stats <- matrix(ncol = k, nrow = length(clust.assess))
cluster.sizes <- matrix(ncol = k, nrow = k)
    for(i in c(1:k)){
  row.clust[i] <- paste("Cluster-", i, " size")
}
    for(i in c(2:k)){
  stats.names[i] <- paste("Test", i-1)

  for(j in seq_along(clust.assess)){
    output.stats[j, i] <- unlist(cluster.stats(d = dist, clustering = cutree(tree, k = i))[clust.assess]

  }

  for(d in 1:k) {
    cluster.sizes[d, i] <- unlist(cluster.stats(d = dist, clustering = cutree(tree, k = i))[clust.size]
    dim(cluster.sizes[d, i]) <- c(length(cluster.sizes[i]), 1)
    cluster.sizes[d, i]

  }
}
    output.stats.df <- data.frame(output.stats)
    cluster.sizes <- data.frame(cluster.sizes)
cluster.sizes[is.na(cluster.sizes)] <- 0
    rows.all <- c(clust.assess, row.clust)
output <- rbind(output.stats.df, cluster.sizes)[ ,-1]
colnames(output) <- stats.names[2:k]
rownames(output) <- rows.all
is.num <- sapply(output, is.numeric)
output[is.num] <- lapply(output[is.num], round, 2)
output
}
```

```
stats.df.agglm <-cstats.table(gower.dist, aggl.clust.m, 8)
stats.df.agglm
```

```
##                     Test 1 Test 2 Test 3 Test 4 Test 5 Test 6 Test 7
## cluster.number        2.00   3.00   4.00   5.00   6.00   7.00   8.00
## n                   528.00 528.00 528.00 528.00 528.00 528.00 528.00
## within.cluster.ss    26.88  21.69  13.37  11.75  11.56   9.31   6.87
## average.within        0.28   0.25   0.19   0.18   0.18   0.16   0.13
## average.between       0.51   0.50   0.45   0.45   0.45   0.44   0.43
## wb.ratio              0.55   0.49   0.42   0.40   0.39   0.35   0.31
## dunn2                 1.68   1.56   1.65   1.67   1.53   1.45   1.45
## avg.silwidth          0.43   0.41   0.44   0.45   0.45   0.43   0.48
## Cluster- 1  size    369.00 369.00 157.00 157.00 157.00  72.00  72.00
## Cluster- 2  size    159.00 102.00 102.00  24.00  21.00  21.00  21.00
## Cluster- 3  size      0.00  57.00 212.00 212.00 212.00 212.00 145.00
## Cluster- 4  size      0.00   0.00  57.00  57.00  57.00  85.00  85.00
## Cluster- 5  size      0.00   0.00   0.00  78.00  78.00  57.00  57.00
## Cluster- 6  size      0.00   0.00   0.00   0.00   3.00  78.00  67.00
## Cluster- 7  size      0.00   0.00   0.00   0.00   0.00   3.00  78.00
## Cluster- 8  size      0.00   0.00   0.00   0.00   0.00   0.00   3.00
```

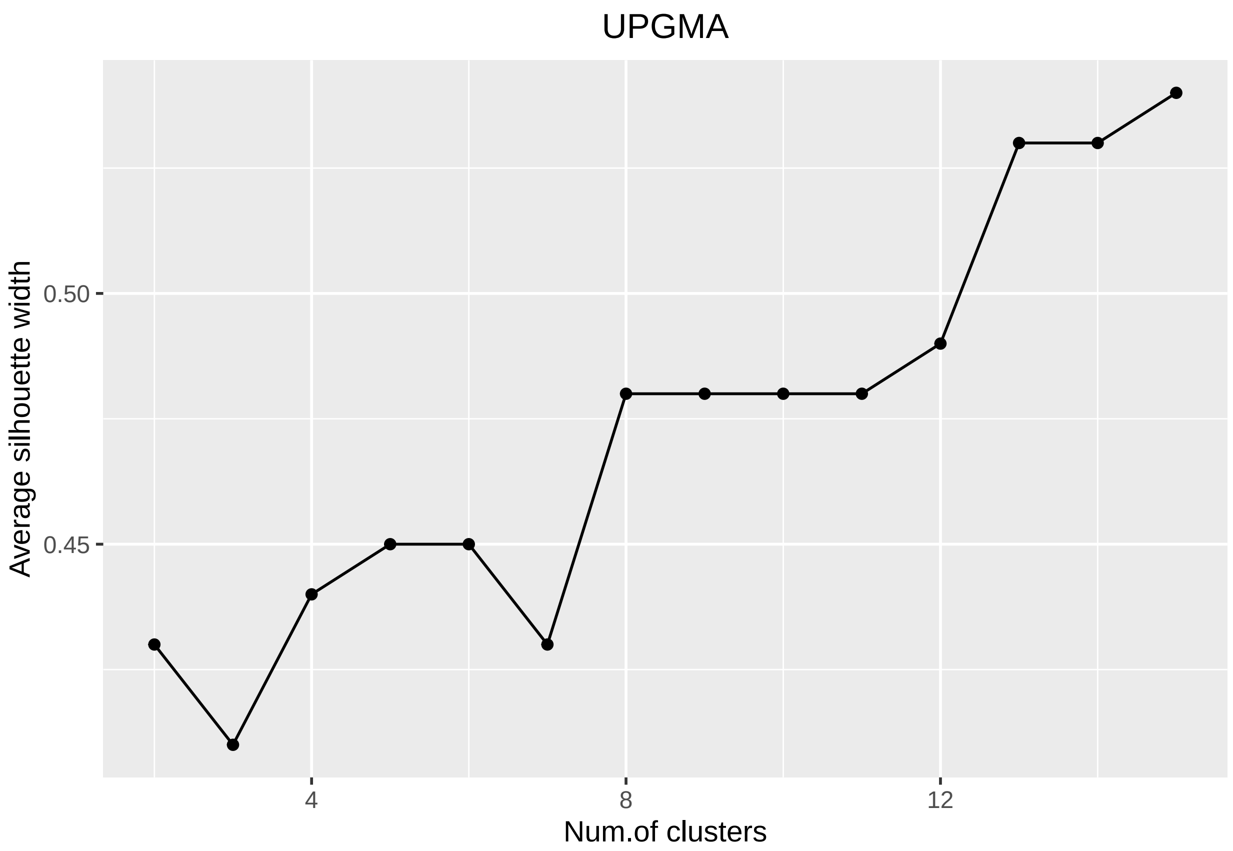
Elbow visualization

```
ggplot(data = data.frame(t(cstats.table(gower.dist, aggl.clust.m, 15))),
  aes(x=cluster.number, y=within.cluster.ss)) +
  geom_point()+
  geom_line()+
  ggtitle("UPGMA") +
  labs(x = "Num.of clusters", y = "Within clusters sum of squares (SS)") +
  theme(plot.title = element_text(hjust = 0.5))
```



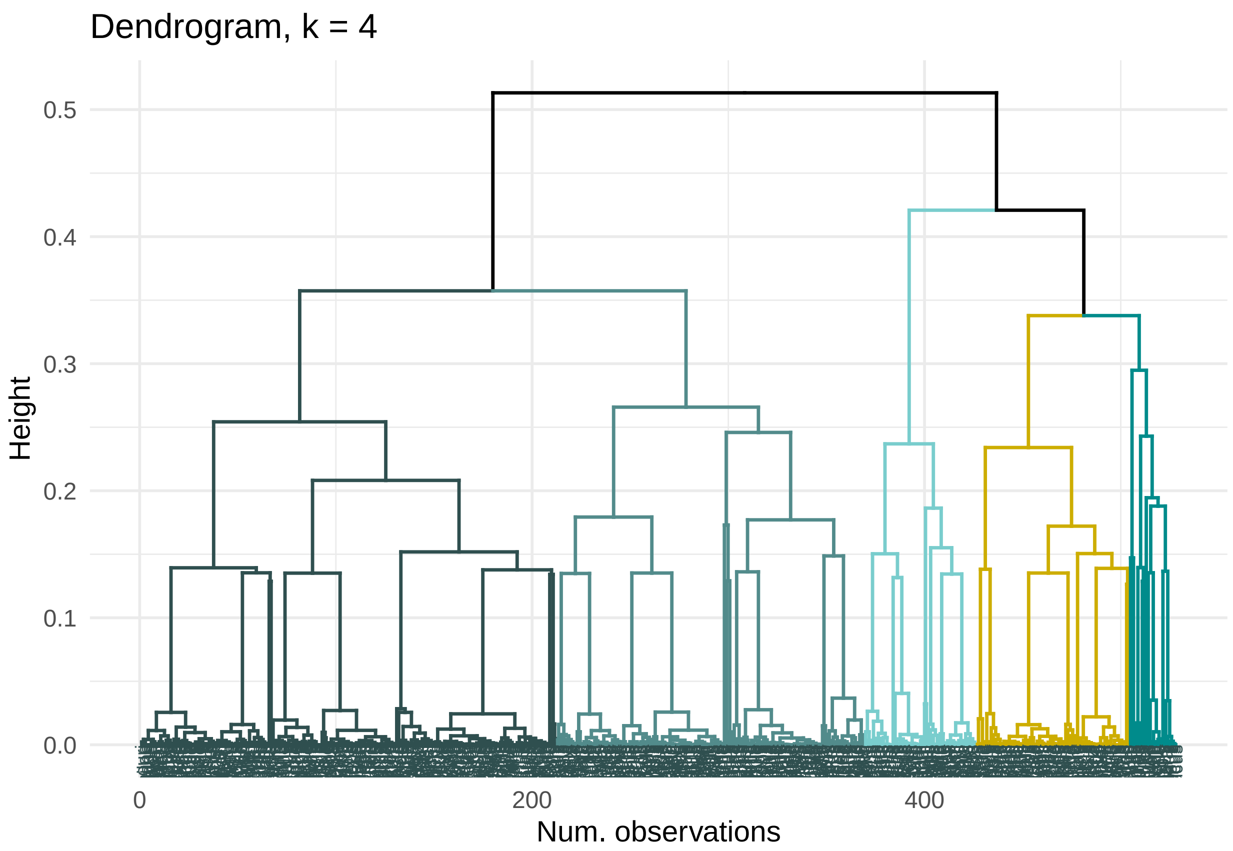
Silhouette visualization

```
ggplot(data = data.frame(t(cstats.table(gower.dist, aggl.clust.m, 15))),
  aes(x=cluster.number, y=avg.silwidth)) +
  geom_point()+
  geom_line()+
  ggtitle("UPGMA") +
  labs(x = "Num.of clusters", y = "Average silhouette width") +
  theme(plot.title = element_text(hjust = 0.5))
```



Dendrogramme visualization

```
dendro <- as.dendrogram(aggl.clust.m)
dendro.col <- dendro %>%
  set("branches_k_color", k = 5, value =   c("darkslategray", "darkslategray4", "darkslategray3", "gold3
  set("branches_lwd", 0.6) %>%
  set("labels_colors",
      value = c("darkslategray")) %>%
  set("labels_cex", 0.5)
ggd1 <- as.ggdend(dendro.col)
ggplot(ggd1, theme = theme_minimal()) +
  labs(x = "Num. observations", y = "Height", title = "Dendrogram, k = 4")
```



```
### Clearly indicates 5 groups
```

Traits & repartition for optimal group number

```
clust.num <- cutree(aggl.clust.m, k = 5)
df<-cbind(df1, clust.num)
df<-as.data.frame(unclass(df),stringsAsFactors=TRUE)
summary(df[df[,length(df[1,])]== 1,])
```

```
##  Reproduction Lower.Slope.Deep Upper.Slope Shelf      Reef     Coastal
##  O :52        No :135          No :69      No :  0   No :157   No :152
##  Oo: 3        Yes: 22          Yes:88      Yes:157   Yes:  0   Yes:  5
##  PV:16
##  YV:86
##
##
##  Oceano.Pelagic   body_size       clust.num
##  No :156        Min.   :3.497   Min.   :1
##  Yes:  1        1st Qu.:4.143   1st Qu.:1
##                 Median :4.615   Median :1
##                 Mean   :4.609   Mean   :1
##                 3rd Qu.:5.011   3rd Qu.:1
##                 Max.   :6.628   Max.   :1
```

```
summary(df[df[,length(df[1,])]== 2,])
```

```
##  Reproduction Lower.Slope.Deep Upper.Slope Shelf     Reef     Coastal
##  O : 0        No :24           No :20      No : 2   No :19   No : 1
##  Oo:12        Yes: 0           Yes: 4      Yes:22   Yes: 5   Yes:23
##  PV:10
##  YV: 2
##
##
##  Oceano.Pelagic   body_size       clust.num
##  No : 0         Min.   :4.477   Min.   :2
##  Yes:24         1st Qu.:5.712   1st Qu.:2
##                 Median :6.058   Median :2
##                 Mean   :6.036   Mean   :2
##                 3rd Qu.:6.369   3rd Qu.:2
##                 Max.   :7.496   Max.   :2
```

```
summary(df[df[,length(df[1,])]== 3,])
```

```
##  Reproduction Lower.Slope.Deep Upper.Slope Shelf      Reef     Coastal
##  O : 90       No : 67          No : 58     No :212   No :212   No :212
##  Oo:  4       Yes:145          Yes:154     Yes:  0   Yes:  0   Yes:  0
##  PV:  2
##  YV:116
##
##
##  Oceano.Pelagic   body_size       clust.num
##  No :212        Min.   :2.639   Min.   :3
##  Yes:  0        1st Qu.:3.738   1st Qu.:3
##                 Median :4.060   Median :3
##                 Mean   :4.058   Mean   :3
##                 3rd Qu.:4.431   3rd Qu.:3
##                 Max.   :5.136   Max.   :3
```

```
summary(df[df[,length(df[1,])]== 4,])
```

```
##  Reproduction Lower.Slope.Deep Upper.Slope Shelf     Reef    Coastal
##  O :40        No :57           No :55      No :50   No : 0   No :27
##  Oo: 0        Yes: 0           Yes: 2      Yes: 7   Yes:57   Yes:30
##  PV: 0
##  YV:17
##
##
##  Oceano.Pelagic   body_size       clust.num
##  No :57         Min.   :3.761   Min.   :4
##  Yes: 0         1st Qu.:4.248   1st Qu.:4
##                 Median :4.466   Median :4
##                 Mean   :4.564   Mean   :4
##                 3rd Qu.:4.787   3rd Qu.:4
##                 Max.   :5.869   Max.   :4
```

```
summary(df[df[,length(df[1,])]== 5,])
```

```
##  Reproduction Lower.Slope.Deep Upper.Slope Shelf     Reef    Coastal
##  O : 0        No :78           No :78      No :14   No :51   No : 0
##  Oo: 1        Yes: 0           Yes: 0      Yes:64   Yes:27   Yes:78
##  PV:66
##  YV:11
##
```

```
##
##  Oceano.Pelagic   body_size       clust.num
##  No :78         Min.   :4.174   Min.   :5
##  Yes: 0         1st Qu.:4.625   1st Qu.:5
##                 Median :5.011   Median :5
##                 Mean   :5.045   Mean   :5
##                 3rd Qu.:5.451   3rd Qu.:5
##                 Max.   :5.914   Max.   :5
```

Saving data

```
write.table(df, "Trait_syndrom_tab.tsv", sep ="\t")
```