R Programming as a Part of Bigdata Course
Clustering

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23 February 2017

Examples on Clustering Preparation Steps

```
# Step 1: Choose appropriate attributes.
# Step 2: Scale the data.
# Step 3: Screen for outliers.
# Step 4: Calculate distances.
# Step 5: Select a clustering algorithm.
#    Hierarchical and/or partitioning cluster analysis.
# Step 5: Repeat using outlier substitution with median.
# Step 5: Repeat using "single" link clustering.
# Step 6: Obtain one or more cluster solutions.
# Step 7: Determine the number of clusters present.
# Step 8: Obtain final clustering solution.
# Step 9: Visualize the results.
```

Examples on References of Relevance to Clustering

- The main reference is [Kabacoff, 2015] Chap. 16 "Clustering Analysis"
- and a selection of R packages and their corresponding bagground papers typical in Journal of Statistical Software,
- e.g. [Charrad, 2014] NbClust: An R Package for Determining the Relevant Number of Clusters in a Data Set
- and [Pison, 1999] Displaying a Clustering with CLUSPLOT, from Elsevier.

Choose Attributes

```
> # 5.1: Step 1: Choose appropriate attributes.
> # Example p. 373 [Kabacoff, 2015]
> data(nutrient, package="flexclust")
> str(nutrient)
'data.frame': 27 obs. of  5 variables:
 $ energy : int  340 245 420 375 180 115 170 160 265 300 ...
 $ protein: int  20 21 15 19 22 20 25 26 20 18 ...
 $ fat    : int  28 17 39 32 10 3 7 5 20 25 ...
 $ calcium: int  9 9 7 9 17 8 12 14 9 9 ...
 $ iron   : num  2.6 2.7 2 2.6 3.7 1.4 1.5 5.9 2.6 2.3 ...
> head(nutrient, 3) # Display upper 3 rows from 5 dim. DS
                 energy protein fat calcium iron
BEEF BRAISED        340      20  28       9  2.6
HAMBURGER           245      21  17       9  2.7
BEEF ROAST          420      15  39       7  2.0
```

Scale Attributes

```
#########################################################
# 5.2: Step 2: Scale the data.
#
# Scaling: For each attribute (variable):
#  Compute mean value, subtract mean value => mean = 0
#  Compute spread, normalize with spread => variance = 1
#      The data scaling is included in Step. 5.
#
```

Scale Attributes

```
#############################################################
# 5.3: Step 3: Screen for outliers.
#      This step is exemplified using ref. [Filzmoser, 2005].
#
# Ref. [Kabacoff, 2015] p. 371
# screen and remove univariate outliers using package: outliers
# install.packages("outliers") # Moved to top of this script.
# install.packages("mvoutlier") # Moved to top of this script.
# library(outliers)
# library(mvoutlier)
# help(package="outliers")    # Single variable outliers.
# help(package="mvoutliers")  # Multivariable outliers.
#
```

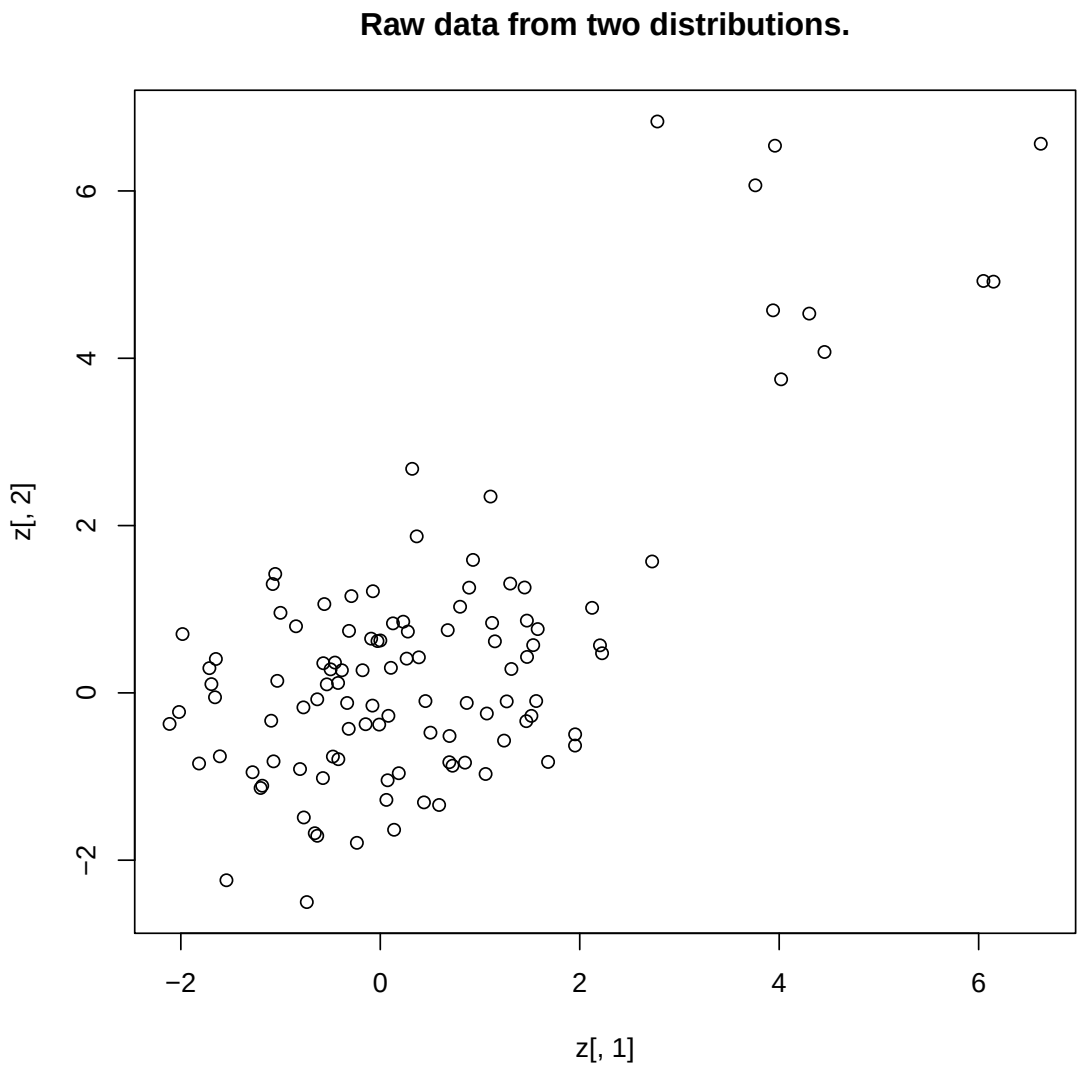
Scale Attributes

```
# ref. [Filzmoser, 2005], package "mvoutliers"
# Demonstrate the function symbol.plot()
# Objective:
# A method for multivariate outlier detection able
# to distinguish between extreme values of a normal
# distribution and values originating from a different
# distribution (outliers).
# Method: Find subset of observations, h, with
# MCD (Minimum Covariance Determinant).
#
```

Scale Attributes

```
# Create data matrices with two different distributions:
# Matrix x: Two column vectors with 100 rows of std. normal.
x <- cbind(rnorm(100), rnorm(100))
# Matrix y: Two column vectors 10 rows of norm. mean=5, std=1
y <- cbind(rnorm(10, 5, 1), rnorm(10, 5, 1))
# Matrix z: Two column vectors, each with 110 rows.
z <- rbind(x,y)
str(z)        # Check structure of resulting z matrix
head(z, 10)  # Check the top 20 rows in z.
par(opar.org)
plot(z[,1],z[,2])
title("Raw data from two distributions.")
```

Raw data for outlier detection experiment.



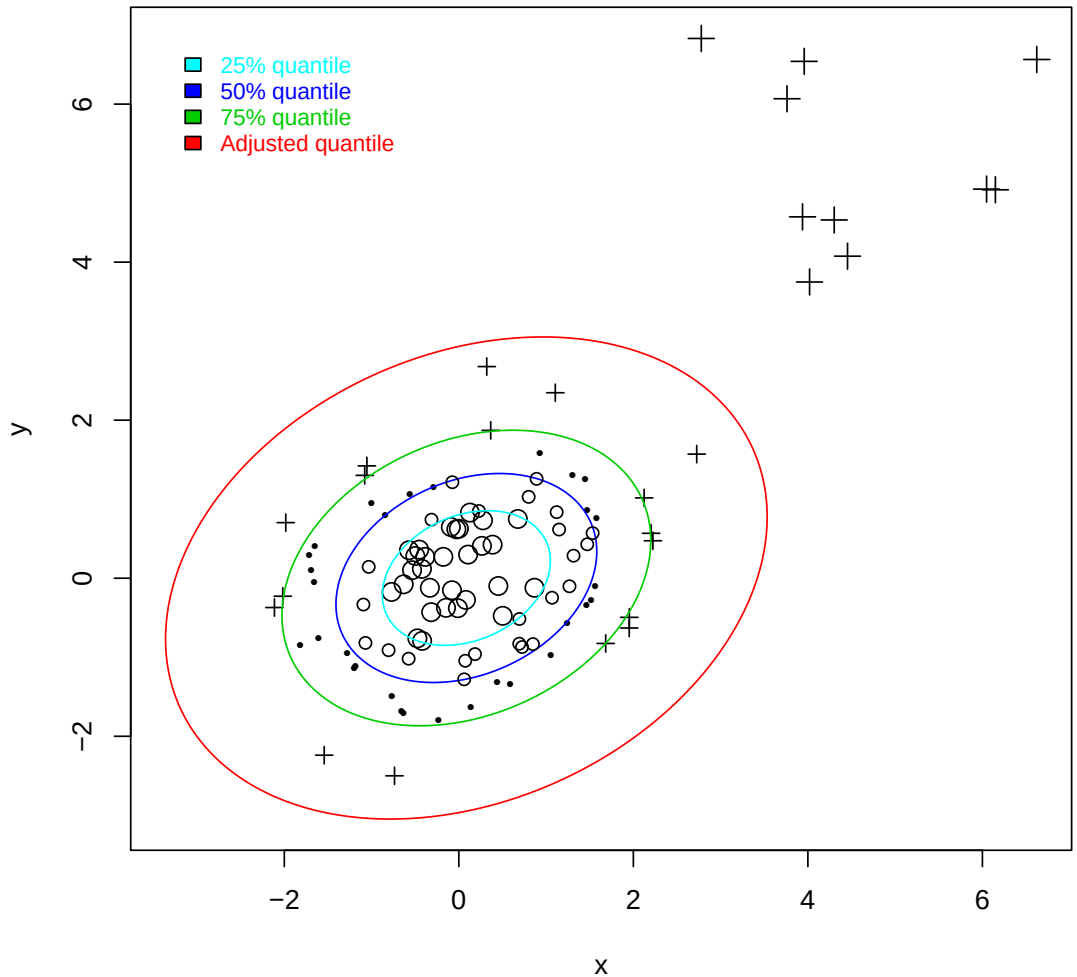
Boolean with outlier True, False

```
> symbol.plot(z, quan=0.75)
$outliers
[1] FALSE FALSE FALSE FALSE FALSE FALSE ...
[20] FALSE FALSE FALSE FALSE FALSE FALSE ...
[39] FALSE FALSE FALSE FALSE FALSE FALSE ...
[58] FALSE FALSE FALSE FALSE FALSE FALSE ...
[77] FALSE FALSE FALSE FALSE FALSE FALSE ...
[96] FALSE FALSE FALSE FALSE FALSE  TRUE
[102] TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE
```

Mahalanobis distance

```
$md
  [1] 1.5488775 0.6202039 0.5959240 2.2306050 ...
 [12] 0.9678372 0.3507535 0.6464982 0.2694994 ...
 .
 .
 .
 [78] 0.3398362 0.9764323 0.5955232 1.5111894 ...
 [89] 2.1523832 1.6060837 1.1749813 1.3489594 ...
[100] 0.3659154 4.0687445 5.7896500 6.9665733 ...
[105] 5.6263406 6.1093877 4.6828475 6.0451329 ...
```

symbol.plot() for outlier removal.



Distance Calculation I

```
#################################################
# 5.4: Step 4: Calculate distances.
#
# Compute dist. matrix btw. first 4 rows of nutrient,
# using the dist() function in R base installation.
# dist() contains the following distances using ?dist()
#        "euclidean", "maximum", "manhattan",
#        "canberra", "binary", "minkowski"
#
?dist()                    # Check manual.
d <- dist(nutrient)        #
as.matrix(d)[1:4,1:4]  # Symm. dist. matrix, 0 diagonal.
#       Notice the very different numerical ranges
#       of the variables => need for scaling.
```

Distance Calculation II

```
> d <- dist(nutrient)
> as.matrix(d)[1:4,1:4]  # Symm. dist. mtx, 0 diagonal.
               BEEF BRAISED HAMBURGER BEEF ROAST BEEF STEAK
BEEF BRAISED      0.00000   95.6400   80.93429   35.24202
HAMBURGER        95.64000    0.0000  176.49218  130.87784
BEEF ROAST       80.93429  176.4922    0.00000   45.76418
BEEF STEAK       35.24202  130.8778   45.76418    0.00000
>
```

Distance Calculation III

```
# If mixed data types:
# binary, nomial (category), ordinal (eg. Likert)
# or continous (e.g. temperature), use e.g. the daisy()
# function in the cluster package.
# Example on packages for clustering on mixed types:
# Functions for agglomerative clustering: agnes()
# Functions for partitionng around medoids: pam().
```

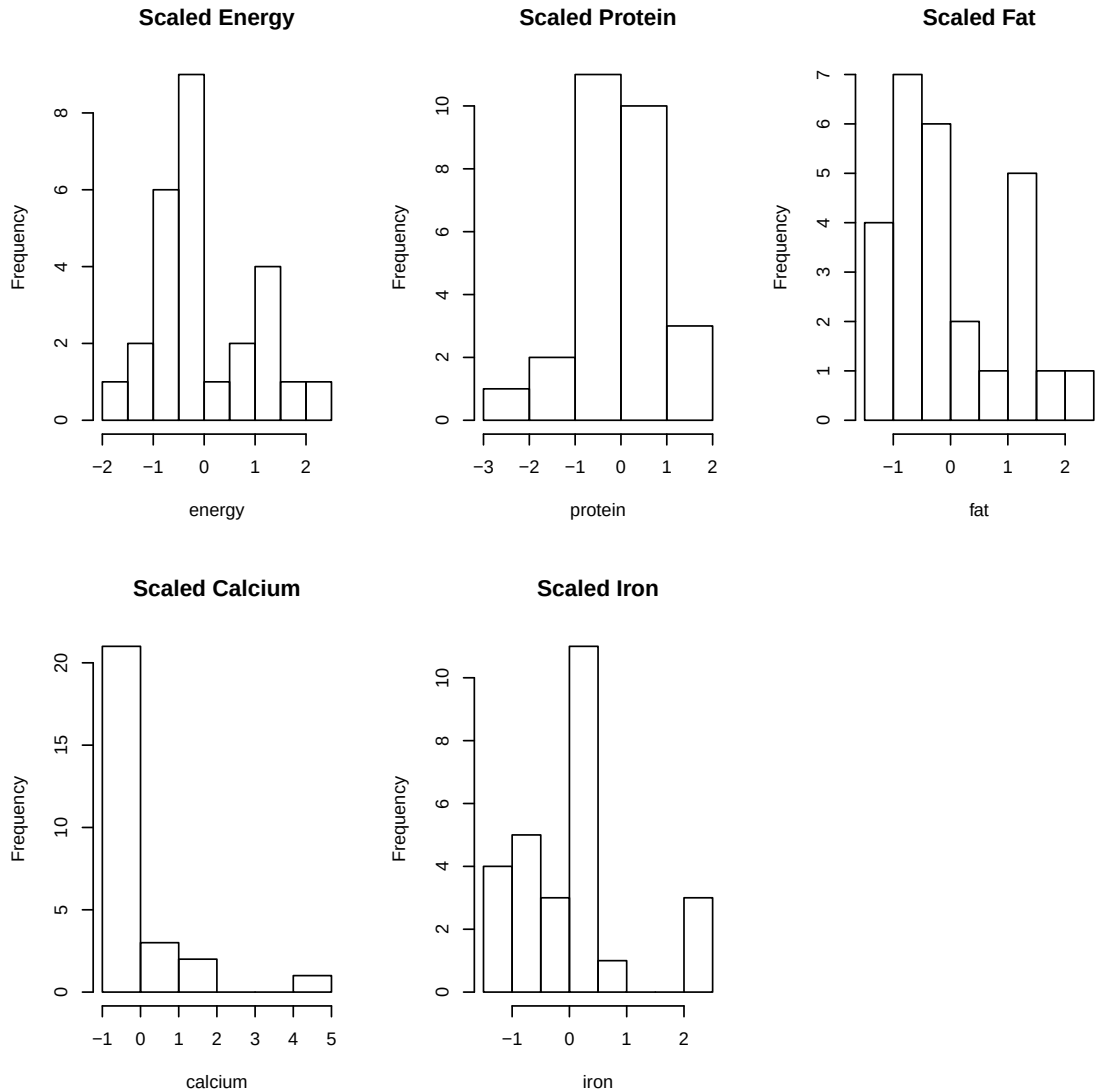
Select a Clustering Algorithm

```
##############################################
# 5.5: Step 5: Select a clustering algorithm.
# Average-linkage clustering of neutrient data.
# Listing 16.1 p. 375 [Kabacoff, 2015.
#
data(nutrient, package="flexclust")
?tolower()            # Check manual.
row.names(nutrient) <- tolower(row.names(nutrient))
?scale()              # Check manual for the scaling function.
nutrient.scaled <- scale(nutrient) # Scale all variables to
                                   #  mean = 0 and spread = 1.
```

Verify Scaling of the Attributes

```
# Check the scaled variables properties.
#    Mean values = 0
#    Standard deviations = 1.
#
attributes(nutrient.scaled)
# Verify that mean values are = 0.
summary(nutrient.scaled)
```

Scaled Histograms of Attributes for Clustering



Euclidean Distance Matrix for scaled nutrient

```
#
# Display the euclidean distance matrix of
#  nutrient.scaled
#
?dist()       # Manual for dist()
d_eucli <- dist(nutrient.scaled,"euclidean")
d_eucli
#
```

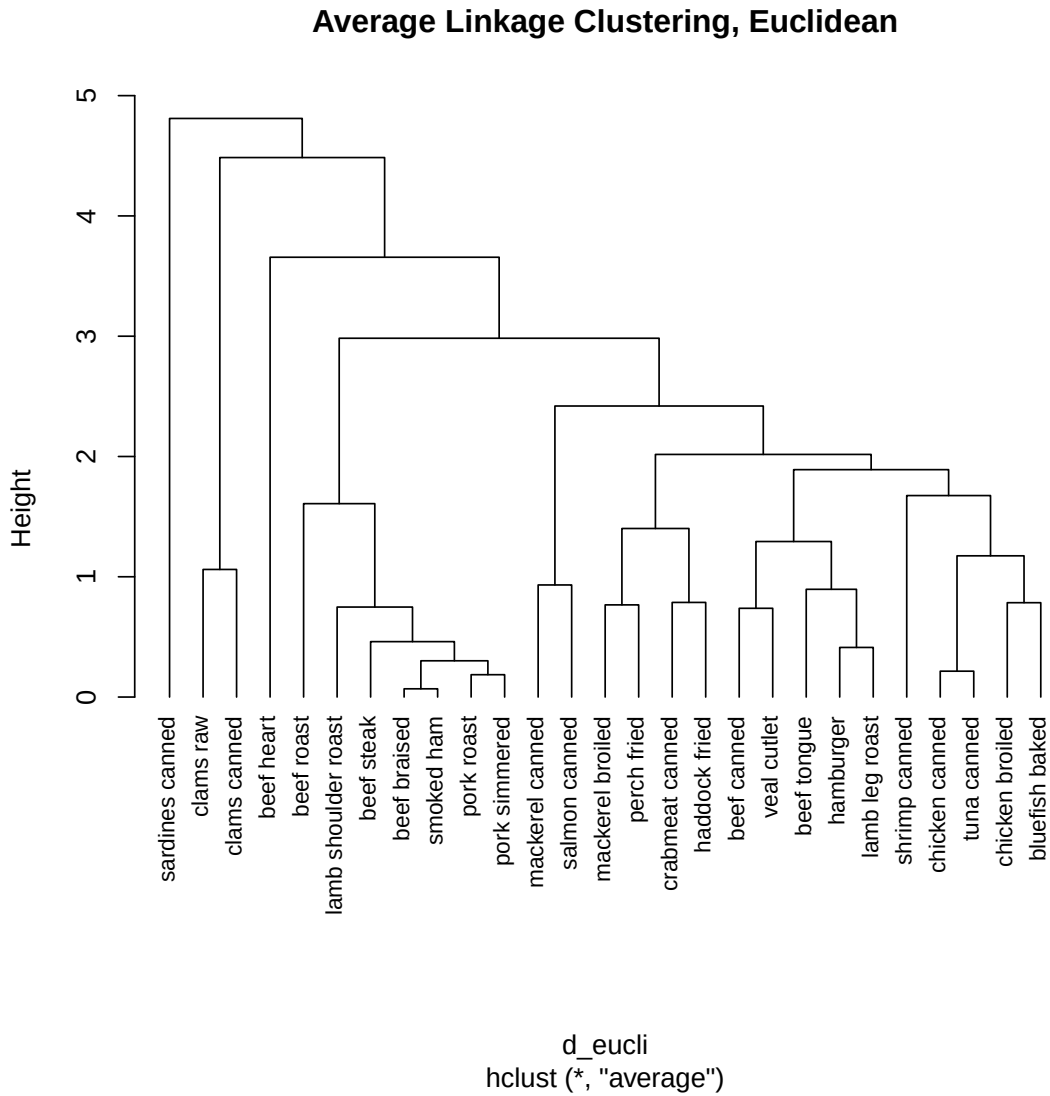
Check Attributes of Dataset in d_eucli

```
> attributes(d_eucli)
$Size
[1] 27

$Labels
[1] "beef braised"          "hamburger"      ...
[5] "beef canned"           "chicken broiled"  ...
[9] "lamb leg roast"        "lamb shoulder roast" ...
[13] "pork simmered"         "beef tongue"  ...
[17] "clams raw"             "clams canned"  ...
[21] "mackerel broiled"      "mackerel canned" ...
[25] "sardines canned"       "tuna canned"  ...
#
```

Average Link Clustering, Euclidean Distance

```
par(opar)
fit.average_eucli <- hclust(d_eucli, method="average")
plot(fit.average_eucli, hang=-1, cex=0.8,
     main="Average Linkage Clustering, Euclidean")
# hang=-1, the labels are below the plot, rotated 90 Degree.
# cex=.8, scale text cx times, [Kabacoff, 2015] p. 53.
#
pdf("fig_5_2_AV_Link_Clust.pdf")
par(opar)
plot(fit.average_eucli, hang=-1, cex=0.8,
     main="Average Linkage Clustering, Euclidean")
par(opar)
dev.off()
```

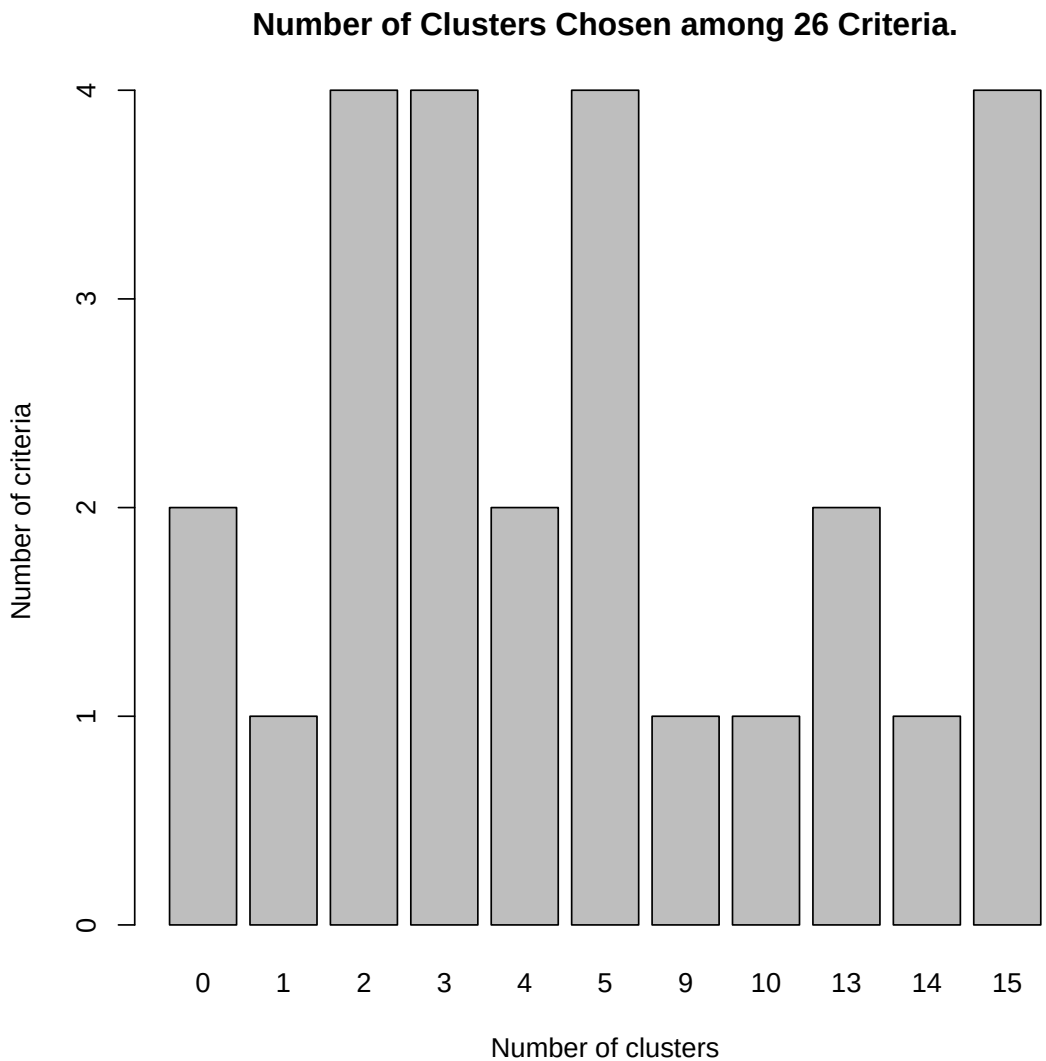
Average Link Clustering, Euclidean Distance



Estimate Number of Clusters

```
par(opar)
nc <- NbClust(nutrient.scaled, distance="euclidean",
              min.nc=2, max.nc=15, method="average")
table(nc$Best.n[1,])
barplot(table(nc$Best.n[1,]),
        xlab="Number of clusters", ylab="Number of criteria",
        main="Number of Clusters Chosen among 26 Criteria.")
par(opar)
#
```

Estimation of the Number of Clusters



Estimation of the Number of Clusters, [Charrad, 2014]

	Name of the index in **NbClust**	Optimal number of clusters
1.	`"ch"` (Calinski and Harabasz 1974)	Maximum value of the index
2.	`"duda"` (Duda and Hart 1973)	Smallest number of clusters such that index > criticalValue
3.	`"pseudot2"` (Duda and Hart 1973)	Smallest number of clusters such that index < criticalValue
4.	`"cindex"` (Hubert and Levin 1976)	Minimum value of the index
5.	`"gamma"` (Baker and Hubert 1975)	Maximum value of the index
6.	`"beale"` (Beale 1969)	Number of clusters such that critical value >= alpha
7.	`"ccc"` (Sarle 1983)	Maximum value of the index
8.	`"ptbiserial"` (Milligan 1980, 1981)	Maximum value of the index
9.	`"gplus"` (Rohlf 1974; Milligan 1981)	Minimum value of the index
10.	`"db"` (Davies and Bouldin 1979)	Minimum value of the index
11.	`"frey"` (Frey and Van Groenewoud 1972)	Cluster level before index value < 1.00
12.	`"hartigan"` (Hartigan 1975)	Maximum difference between hierarchy levels of the index
13.	`"tau"` (Rohlf 1974; Milligan 1981)	Maximum value of the index
14.	`"ratkowsky"` (Ratkowsky and Lance 1978)	Maximum value of the index
15.	`"scott"` (Scott and Symons 1971)	Maximum difference between hierarchy levels of the index
16.	`"marriot"` (Marriot 1971)	Max. value of second differences between levels of the index
17.	`"ball"` (Ball and Hall 1965)	Maximum difference between hierarchy levels of the index
18.	`"trcovw"` (Milligan and Cooper 1985)	Maximum difference between hierarchy levels of the index
19.	`"tracew"` (Milligan and Cooper 1985)	Max. value of second differences between levels
20.	`"friedman"` (Friedman and Rubin 1967)	Maximum difference between hierarchy levels of the index
21.	`"mcclain"` (McClain and Rao 1975)	Minimum value of the index
22.	`"rubin"` (Friedman and Rubin 1967)	Minimum value of second differences between levels
23.	`"kl"` (Krzanowski and Lai 1988)	Maximum value of the index
24.	`"silhouette"` (Rousseeuw 1987)	Maximum value of the index
25.	`"gap"` (Tibshirani *et al.* 2001)	Smallest number of clusters such that criticalValue >= 0
26.	`"dindex"` (Lebart *et al.* 2000)	Graphical method
27.	`"dunn"` (Dunn 1974)	Maximum value of the index
28.	`"hubert"` (Hubert and Arabie 1985)	Graphical method
29.	`"sdindex"` (Halkidi *et al.* 2000)	Minimum value of the index
30.	`"sdbw"` (Halkidi and Vazirgiannis 2001)	Minimum value of the index

Table 2: Overview of the indices implemented in the **NbClust** package.

Final Clustering Solution I

```
par(opar)
> # 5.8: Step 8: Obtain final clustering solution.
> #
> # Listing 16.3 page 377 [Kabacoff, 2015]
> #
> ?cutree()    # Manual for tree cutting.
# Use k=5 groups as desired.
> clusters <- cutree(fit.average_eucli, k=5)
> table(clusters)
clusters
 1  2  3  4  5
 7 16  1  2  1
```

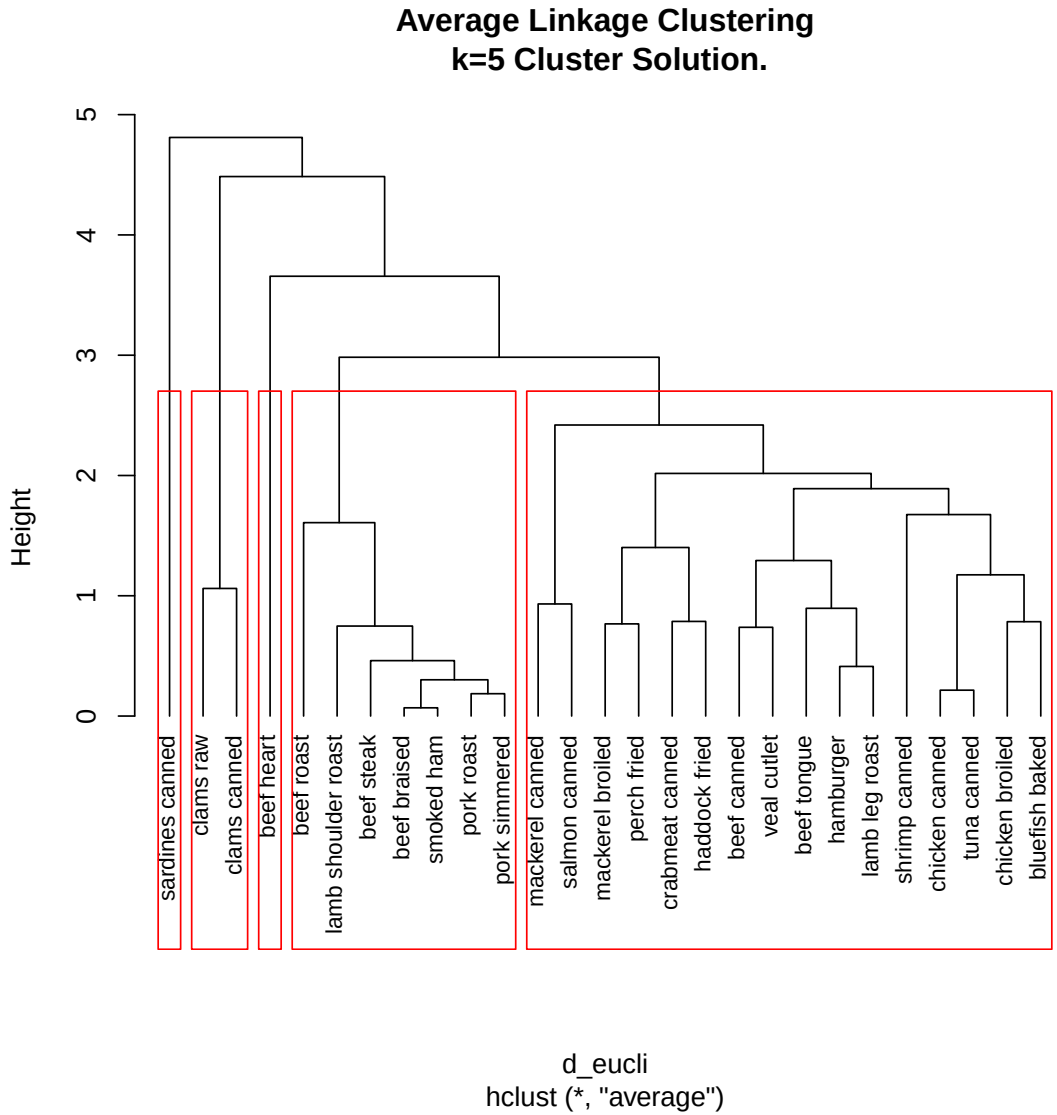
Final Clustering Solution II

```
> aggregate(nutrient, by=list(cluster=clusters), median)
clust energ prote fat calc iron
  1   340.0  19    29   9  2.50
  2   170.0  20     8  13  1.45
  3   160.0  26     5  14  5.90
  4    57.5   9     1  78  5.70
  5   180.0  22     9 367  2.50
> #
> aggregate(as.data.frame(nutrient.scaled),
+ by=list(cluster=clusters), median)
clust energ prote   fat    calc     iron
  1  1.310  0.000  1.378 -0.4480  0.0811
  2 -0.369  0.235 -0.486 -0.3967 -0.6374
  3 -0.468  1.646 -0.753 -0.3839  2.4077
  4 -1.481 -2.352 -1.108  0.4361  2.2709
  5 -0.270  0.705 -0.398  4.1396  0.0811
> #
```

Visualize Final Solution I

```
#
# Listing 16.3 page 377 [Kabacoff, 2015]
#
par(opar)
plot(fit.average_eucli, hang=-1, cex=0.8,
  main="Average Linkage Clustering\n k=5 Cluster Solution.")
# Display the k=5 cluster solution.
rect.hclust(fit.average_eucli, k=5)
#
```

Visualize Final Solution II



Partitioning Clustering k-means

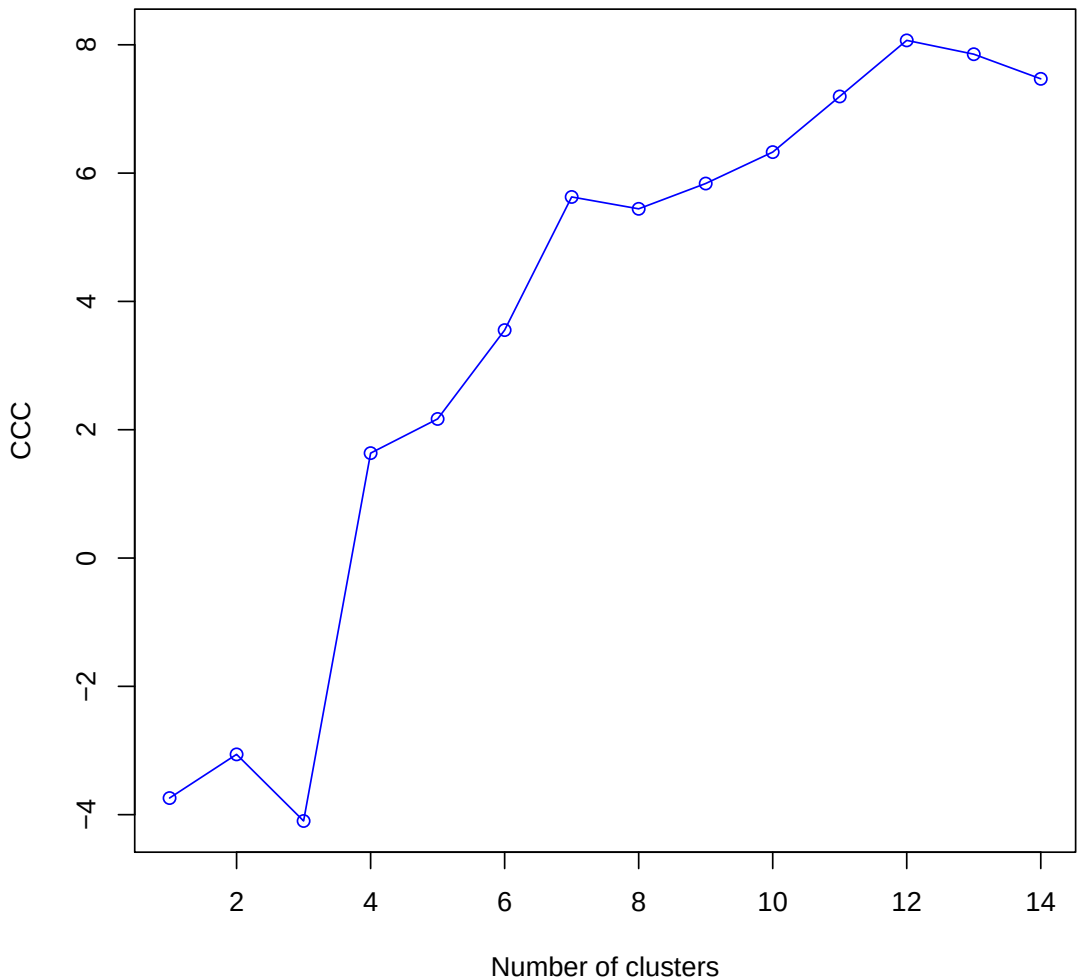
```
########################################################
# 5.20: Examples using the Partitioning Clustering k-means
#
# Ref. page 379 [Kabacoff, 2015] "Plotting function of
#   k-means clusters".
#
# Installed on top of script.
# install.packages("rattle",lib="C:/R_packages/")
# library("rattle",lib="C:/R_packages/")
data(wine, package="rattle")
```

Partitioning Clustering k-means, Dataset: Wine

```
str(wine)
'data.frame': 178 obs. of  14 variables:
 $ Type            : Factor w/ 3 levels "1","2","3": 1 1 1 1 .
 $ Alcohol         : num  14.2 13.2 13.2 14.4 13.2 ...
 $ Malic           : num  1.71 1.78 2.36 1.95 2.59 1.76 1.87 ...
 $ Ash             : num  2.43 2.14 2.67 2.5 2.87 2.45 2.45  ...
 $ Alcalinity      : num  15.6 11.2 18.6 16.8 21 15.2 14.6...
 $ Magnesium       : int  127 100 101 113 118 112 96 121 97 98 ..
 $ Phenols         : num  2.8 2.65 2.8 3.85 2.8 3.27 2.5 2 ...
 $ Flavanoids      : num  3.06 2.76 3.24 3.49 2.69 3. 3.15 ...
 $ Nonflavanoids   : num  0.28 0.26 0.3 0.24 0.39 0.34 0.3 ...
 $ Proanthocyanins: num  2.29 1.28 2.81 2.18 1.82 1.97 1 ...
 $ Color           : num  5.64 4.38 5.68 7.8 4.32 6.75 5. ...
 $ Hue             : num  1.04 1.05 1.03 0.86 1.04 1.0 ...
 $ Dilution        : num  3.92 3.4 3.17 3.45 2.93 2.85 ...
 $ Proline         : int  1065 1050 1185 1480 735 1450 ...
```

The CCC index for the Number of Clusters

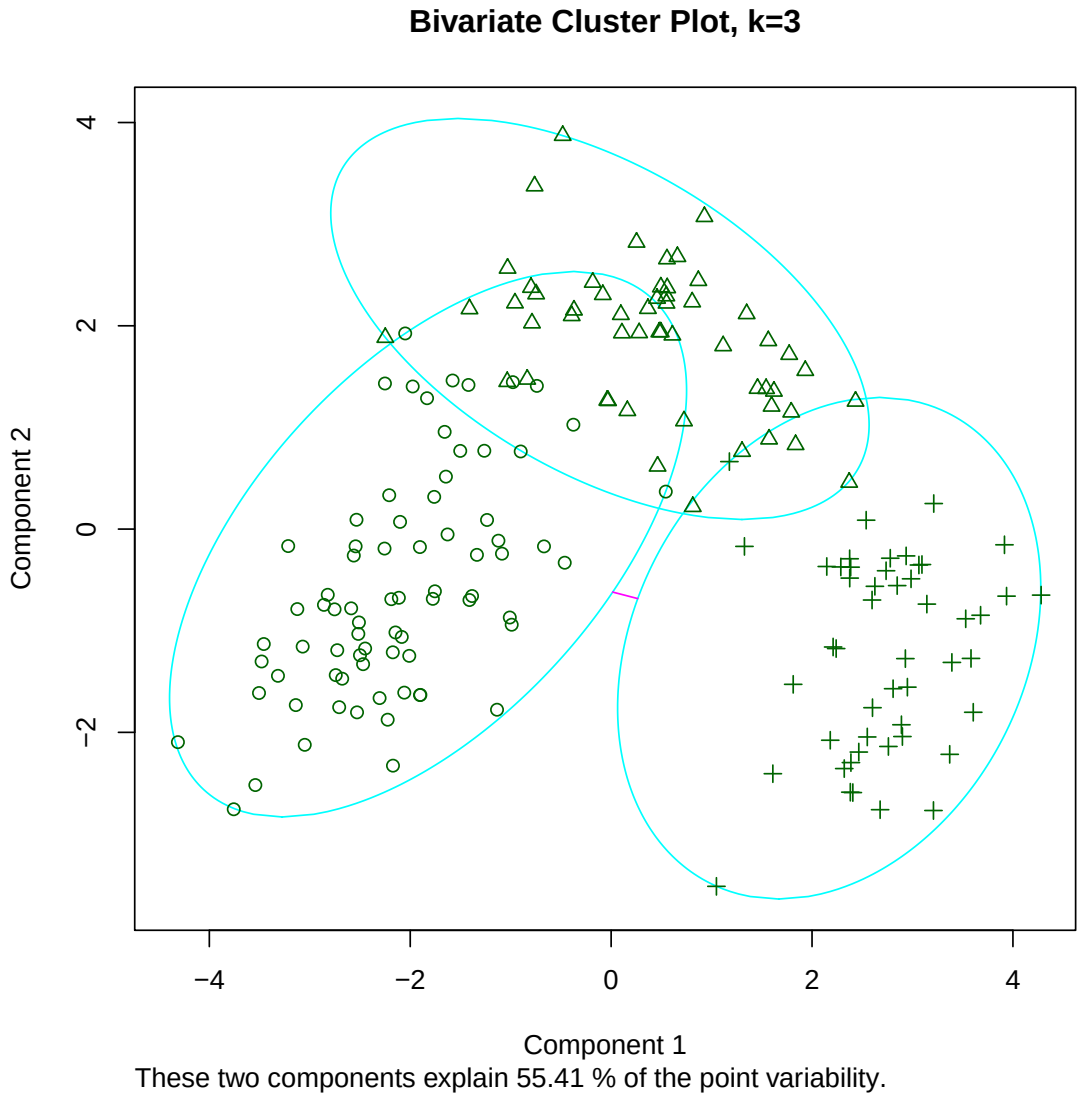
The CCC (Cubic Cluster Criteria) from NbClust() for assessing the quality of the clustering, cf. [Kabacoff, 2015] page 387 and [Charrad, 2014]. If CCC is negative and decreasing for increasing number of clusters, then the dataset has a tendency to unimodality.



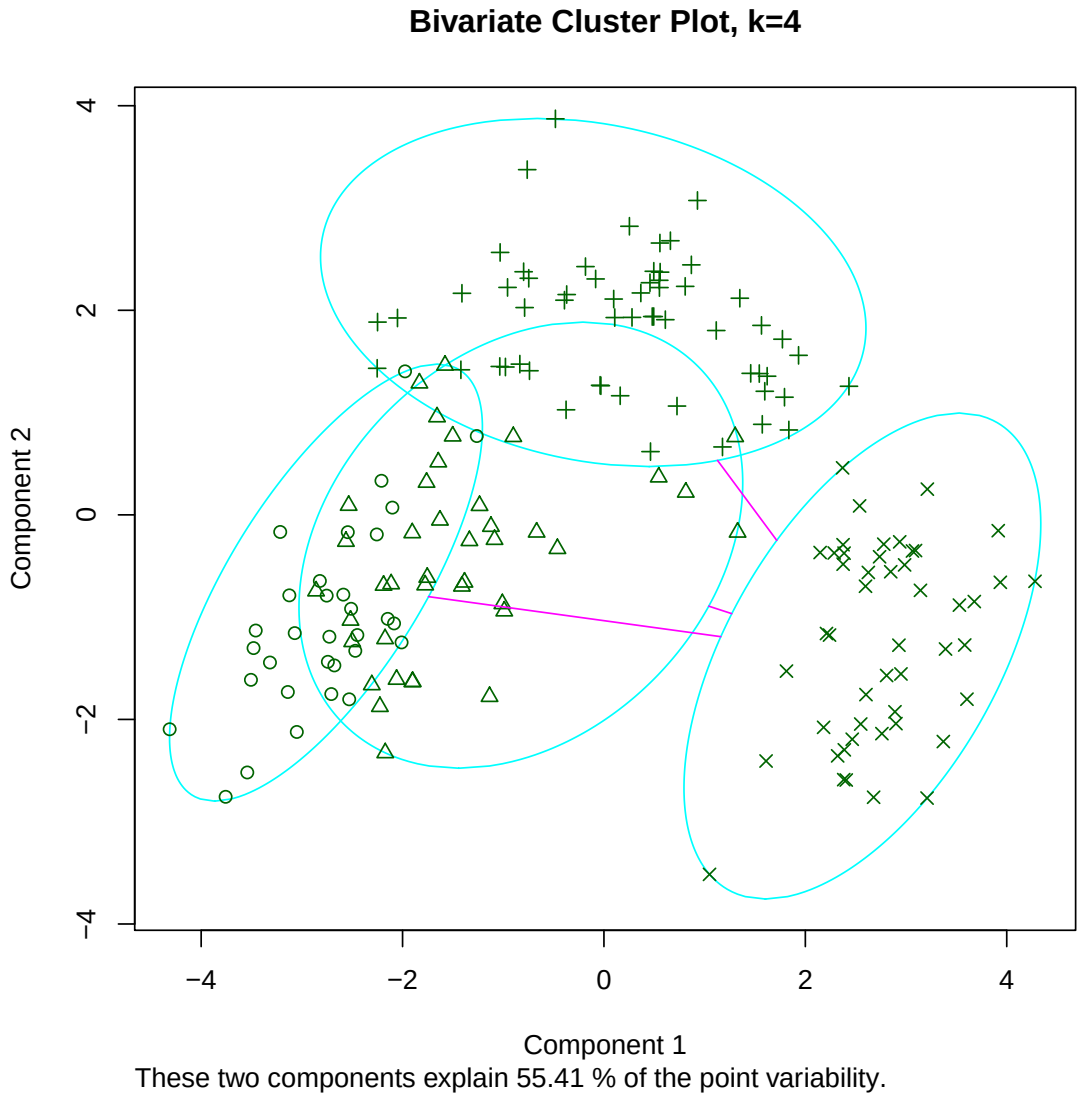
Partitioning around Mediods

```
#####################################################
# 5.30: Examples using the Partitioning around medoids
# Use dataset wine from package rattle
# loaded in section 5.20:  data(wine, package="rattle")
#
# library(cluster) moved to top of script
set.seed(1234)
fit.pam_3 <- pam(wine[-1], k=3, stand=TRUE)
fit.pam_3$medoids
clusplot(fit.pam_3, main="Bivariate Cluster Plot, k=3")
#
```

Partitioning around Medoids, I



Partitioning around Medoids, II



Clustering of mixed variables, Example 1

```
# 5.40: "ClustOfVar" [Cavent, 2012, 2014, 2015].
install.packages("ClustOfVar",lib=loc)
library("ClustOfVar",lib=loc)
# [Chavent, 2011] page 7, Example 1 Quantitative data.
data("decathlon") # 41 Olympic athlets, w. 13 obs. on sports.
str(decathlon)
 'data.frame': 41 obs. of  13 variables:
 $ 100m         : num  11 10.8 11 11 11.3 ...
 $ Long.jump    : num  7.58 7.4 7.6.81 7.56 ...
 $ Shot.put     : num  14.8 14.3 14.8 14.2 15.2 ...
 $ High.jump    : num  2.07 1.86 2.04  1.86 ...
 $ 400m         : num  49.8 49.4 48.4 48.9 50.4 ...
 $ 110m.hurdle: num  14.7 14.1 14.1 15 15.3 ...
 $ Discus       : num  43.8 50.7 49 40.9 46.3 ...
 $ Pole.vault : num  5.02 4.92 4. 4.92 4.82 ...
 $ Javeline     : num  63.2 60.1 50.3 63.4 ...
 $ 1500m        : num  292 302 300 280 276 ...
 $ Rank         : int  1 2 3 4 5 6 7 8 10 ...
 $ Points       : int  8217 8122 7995 7802 7733 ...
 $ Competition: Factor w/ 2 levels "Decastar","OlympicG": 1 1 ..
```

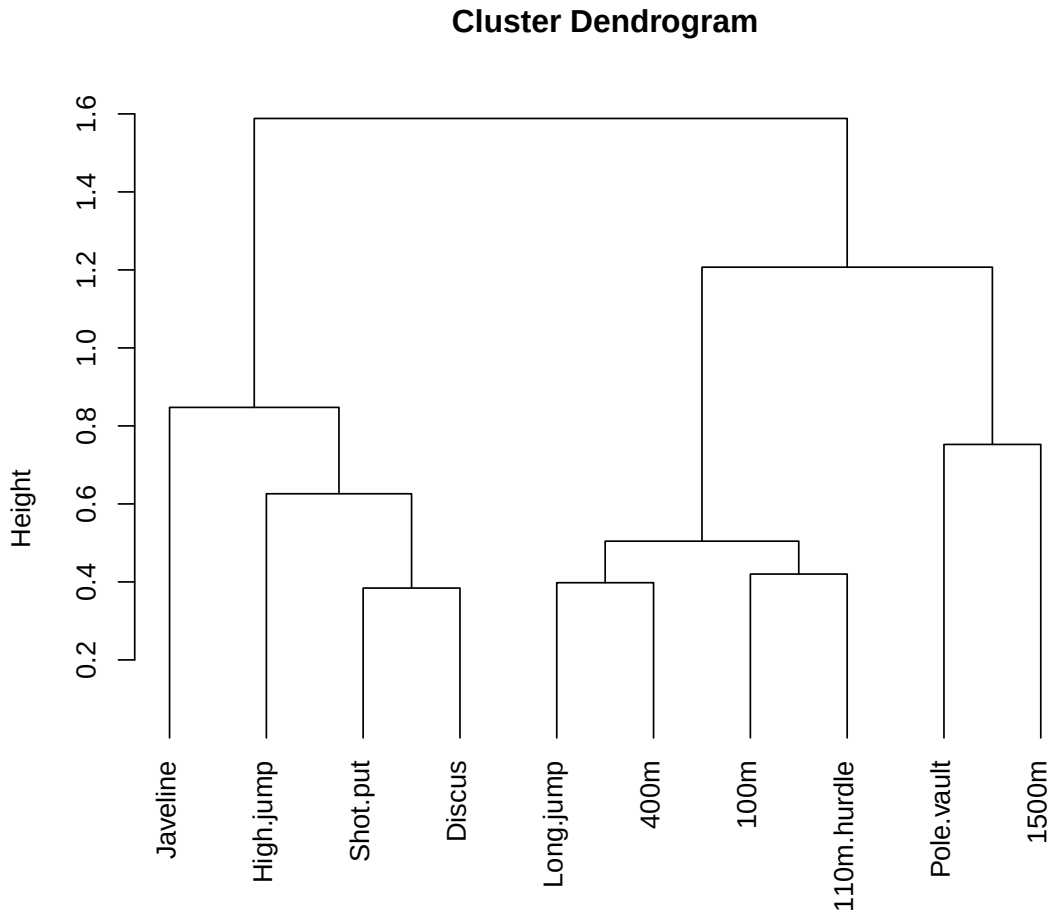
Clustering of mixed variables, Example 1

```
head(decathlon[, 1:4])
          100m Long.jump Shot.put High.jump
SEBRLE   11.04      7.58    14.83      2.07
CLAY     10.76      7.40    14.26      1.86
KARPOV   11.02      7.30    14.77      2.04
BERNARD  11.02      7.23    14.25      1.92
YURKOV   11.34      7.09    15.19      2.10
WARNERS  11.11      7.60    14.31      1.98
```

Clustering of mixed variables, Example 1

```
# Plot dendrogram
tree <- hclustvar(decathlon[, 1:10]) # 10 different sports.
plot(tree)
par(opar.org)
pdf("fig_5_40_1_tree.pdf") # Generate pdf plot.
plot(tree)
dev.off()
par(opar.org)
```

Dendrogram, 10 decathlon sports, Example 1

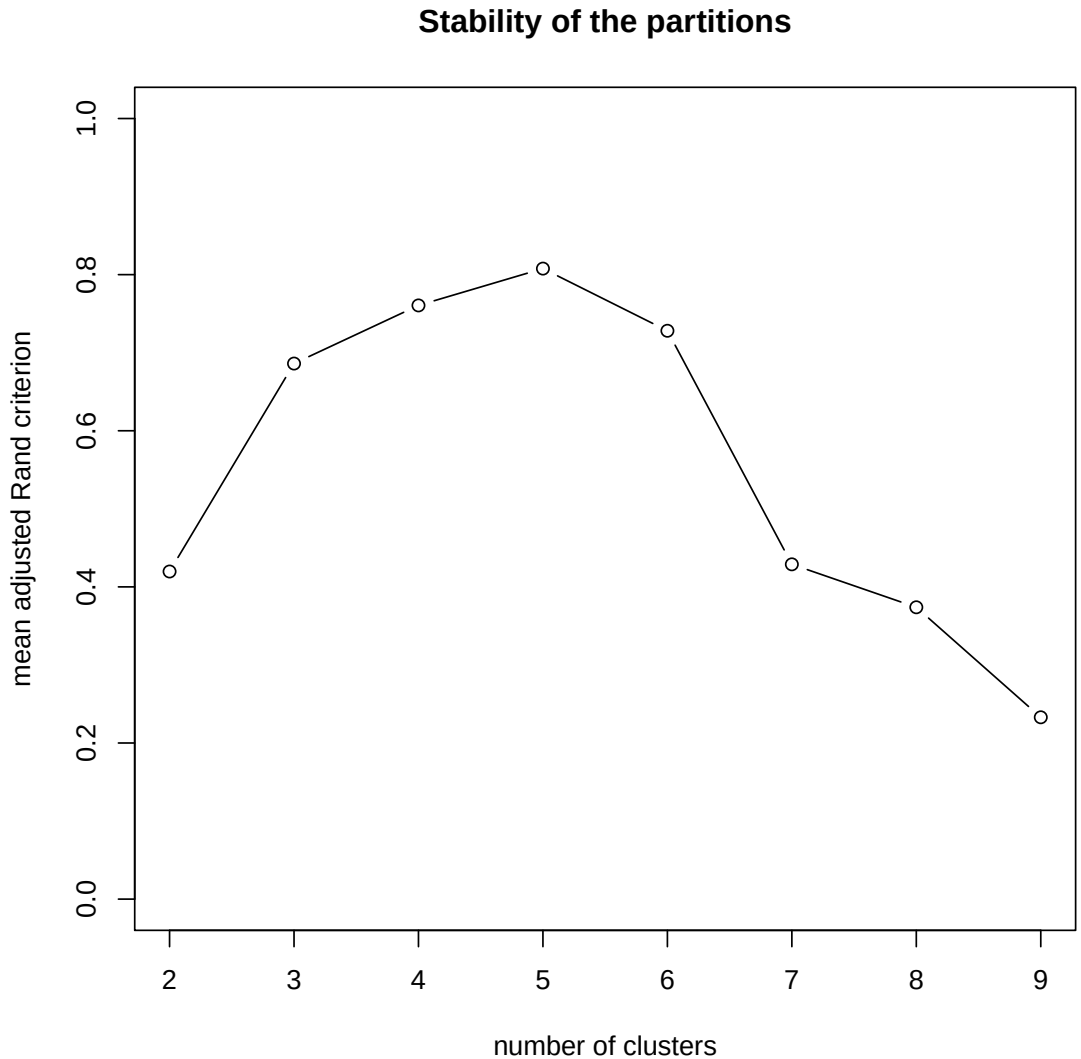


Clustering of mixed variables, Example 1

```
# Check stability of clusters.
stab <- stability(tree, B = 40) # use 40 bootstrap samples.
plot(stab, main = "Stability of the partitions")
par(opar.org)
pdf("fig_5_40_2_Stability.pdf") # Generate pdf plot.
plot(stab, main = "Stability of the partitions")
dev.off()
par(opar.org)
```

Stability of clusters, 10 decathlon sports, Example 1

A high index value signals more stability than a low index value.
The number of bootstrap samples used: B=40.

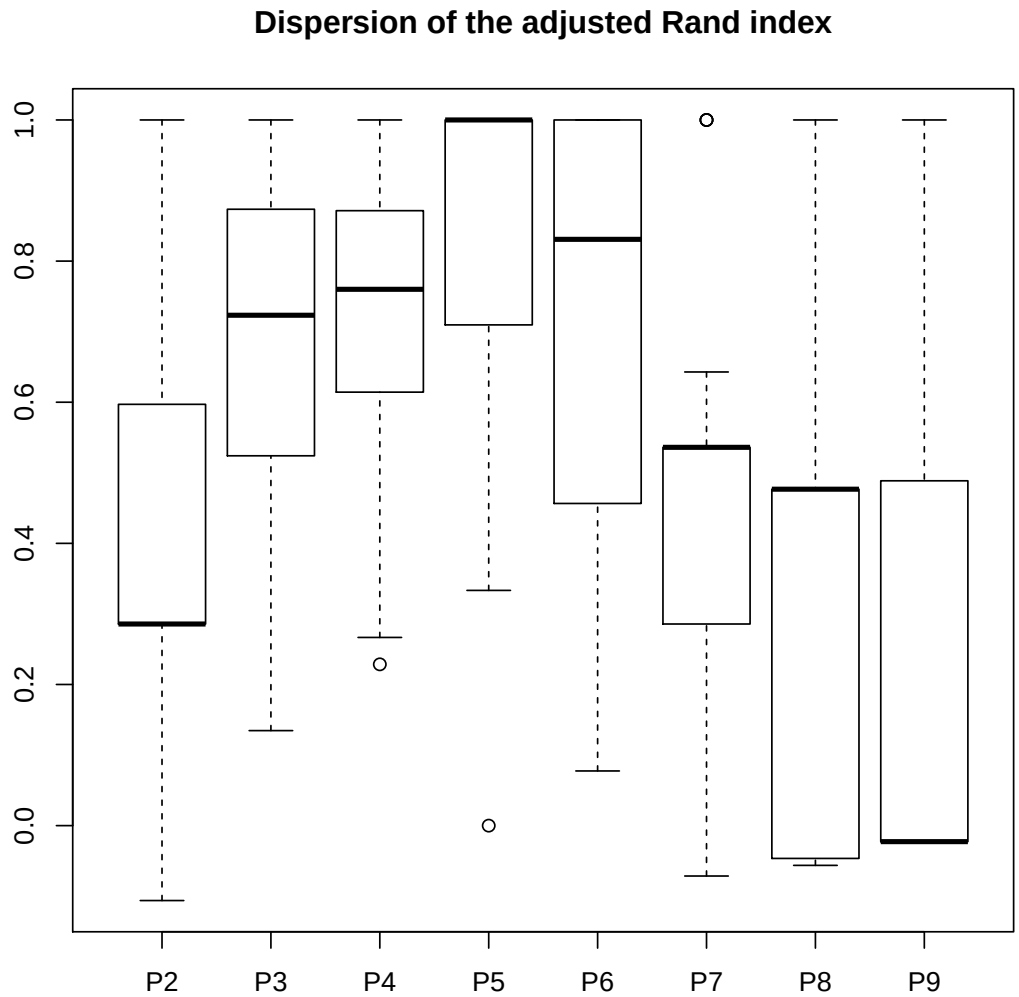


Clustering of mixed variables, Example 1

```
boxplot(stab$matCR, main = "Dispersion of adjusted Rand index")
par(opar.org)
pdf("fig_5_40_3_Boxplot.pdf") # Generate pdf plot.
boxplot(stab$matCR, main = "Dispersion of adjusted Rand index")
dev.off()
par(opar.org)
```

Stability of clusters, 10 decathlon sports, Example 1

The number of bootstraps used: 40.



Clustering of mixed variables, Example 1

```
#
P3 <- cutreevar(tree, 3, matsim = TRUE)
cluster <- P3$cluster
X <- decathlon[, 1:10]
princomp(X[, which(cluster==1)], cor = TRUE)$sdev^2
princomp(X[, which(cluster==2)], cor = TRUE)$sdev^2
princomp(X[, which(cluster==3)], cor = TRUE)$sdev^2
print(P3)
round(P3$sim$cluster1, digit = 2)

P3$cluster

P3$var

head(P3$scores)
```

Clustering of mixed variables, Example 2

```
# ----------------------------------------
# [Chavent, 2012] page 7 -- Example 2 "Mixed Variables".
#
data("wine") # 21 wines (rows)
   # col. 1: Label (3 levels), Col. 2 (4 levels): soil.
   # col. 3-31: Sensory descriptors.
head(wine[, 1:4])
# O.I.b.s: Odor.Intensity.before.shaking
# A.q.b.s: Aroma.quality.before.shaking
          Label      Soil   O.I.b.s  A.q.b.s
2EL      Saumur      Env1     3.074    3.000
1CHA     Saumur      Env1     2.964    2.821
1FON Bourgueuil      Env1     2.857    2.929
1VAU     Chinon      Env2     2.808    2.593
1DAM     Saumur Reference     3.607    3.429
2BOU Bourgueuil Reference     2.857    3.111
```

Clustering of mixed variables, Example 2

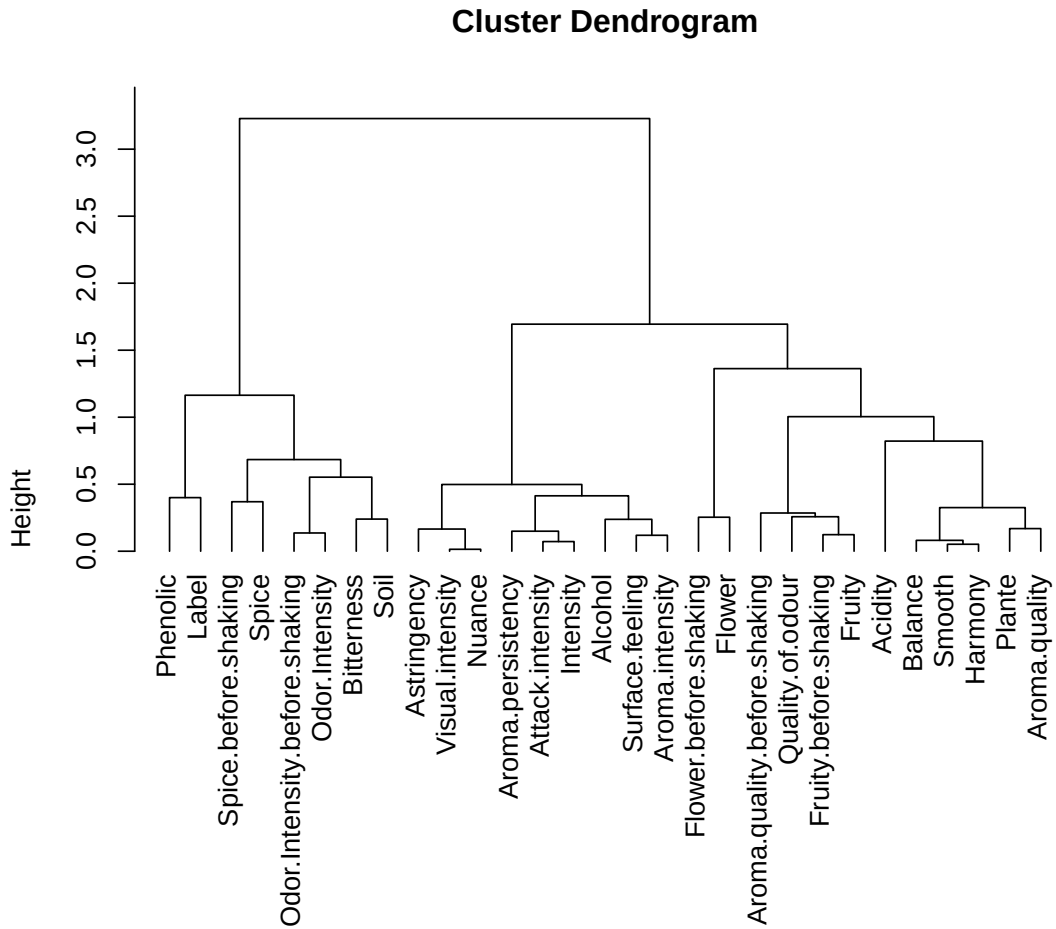
```
str(wine)
'data.frame': 21 obs. of  31 variables:
 $ Label                              : Factor w/ 3 levels ...
 $ Soil                               : Factor w/ 4 levels ...
 $ Odor.Intensity.before.shaking: num  3.07 2.96 2.86 ..
 $ Aroma.quality.before.shaking : num  3 2.82 2.93 2.59 .
 $ Fruity.before.shaking          : num  2.71 2.38 2.56 ...
 $ Flower.before.shaking          : num  2.28 2.28 1.96 ...
 $ Spice.before.shaking           : num  1.96 1.68 2.08 ...
 $ Visual.intensity               : num  4.32 3.22 3.54 ...
 $ Nuance                         : num  4 3 3.39 2.79  ...
 $ Surface.feeling                : num  3.27 2.81 3 2. ...
 $ Odor.Intensity                 : num  3.41 3.37 3.25 ...
 $ Quality.of.odour               : num  3.31 3 2.93 2.8 ...
 $ Fruity                         : num  2.88 2.56 2.77 ...
 ...
 $ Smooth                         : num  2.73 2.5 2.68 ...
 $ Bitterness                     : num  1.93 1.93 2 ...
 $ Overall.quality                : num  3.39 3.21 3.54 ...
 $ Typical                        : num  3.25 3.04 3.18 ...
```

Clustering of mixed variables, Example 2

```
X.quanti <- wine[, 3:29] # 27 quantitative variables.
str(X.quanti)
X.quali <- wine[, 1:2]  # 2  qualitative variables.
str(X.quali)
tree <- hclustvar(X.quanti, X.quali)
plot(tree)
par(opar.org)

pdf("fig_5_40_4_Tree.pdf") # Generate pdf plot.
plot(tree)
dev.off()
par(opar.org)
```

Clustering of mixed variables, Example 2

Using this clustering into 6 groups the origital 21×31 matrix is substituted by an 21×6 matrix. Clustering threshold slightly lower than 1.



Random Forest for variable selection.

```
#############################################################
# 5.50: Ex. using random forest for variable selection
#       in high dimensional data, [Genuer, 2015, 2016].
#
install.packages("ellipse",lib=loc)
install.packages("corpcor",lib=loc)
install.packages("MASS",lib=loc)
install.packages("lattice",lib=loc)
install.packages("ggplot2",lib=loc)
install.packages("mixOmics",lib=loc)
install.packages("VSURF",lib=loc)

library("ellipse",lib=loc)
library("corpcor",lib=loc)
library("MASS",lib=loc)
library("lattice",lib=loc)
library("ggplot2",lib=loc)
library("mixOmics",lib=loc)
library("VSURF",lib=loc)
```

Random Forest for variable selection.

```
# Example Data: toys
#
data("toys")  # toys$x: 100 obs., 200 var.,
    # only 6 dimensions are relevant, the 194 noise.
    # toys$y: 100 obs., 1 var in {-1, +1}
set.seed(3101318)
# Structure of the dataset "toys"
#  ref. [Genuer, 2015], p.23
#  ref. [Weston, 2003], p. 1453.
set.seed(3101318)
# Structure of datset("toys")
# ref. [Genuer, 2015], p.23.
```

Example Dataset Toys I

Using refs. [Genuer, 2015], p. 23 and [Weston, 2003], p. 1453, and [Genuer, 2015], p. 8 defines the Toys dataset as follows:

A dataframe df_X with 100 observations (rows) of 200 input variables (columns).
A dataframe df_Y with the corresponding single column output variable Y, with 100 observations (rows), which is a factor which, with equal probability, assume the values $\{-1, +1\}$.

Thus, in total the data set has 100 observations in 200 dimensions, where
6 dimensions represent information and
194 dimensions represent noise only.

Example Dataset Toys II

Assume that Y is a realization of the single output data frame, with equal probability of the two factor values $\{-1, +1\}$

$$Y = (y_1, y_2, y_3, \ldots, y_j, \ldots, y_{100})$$

Then with probability 0.7

$$X_j \in N(y_j, 1) \text{ for } j = 1, 2, 3 \text{ and } X_j \in N(0, 1) \text{ for } j = 4, 5, 6$$

and with probability 0.3

$$X_j \in N(0, 1) \text{ for } j = 1, 2, 3 \text{ and } X_j \in N(y_{j-3}, 1) \text{ for } j = 4, 5, 6$$

The variables $X_j \in N(0, 1)$ for $j = 7, 8, \ldots, 200$.

Example Dataset Toys III

Alternative representation of the dataset. Notice that

$$N(\mu, \sigma)$$

is a normal probability density with mean μ and spread σ, then

<table>
<tr><th>If $j = 1, 2, 3$</th><th>if $j = 4, 5, 6$</th><th>if $j = 7, \ldots, 200$</th></tr>
<tr><td>then with $prob = 0.7$
$x_j \in N(y_j, 1)$
thus with equal probability
$x_j \in \{N(-1, 1), N(1, 1)\}$</td><td>then with $prob = 0.7$
$x_j \in N(0, 1)$</td><td rowspan="2">then noise only
$x_j \in N(0, 1)$</td></tr>
<tr><td>then with $prob = 0.3$
$x_j \in N(0, 1)$</td><td>then with $prob = 0.3$
$x_j \in N(y_{j-3}, 1)$
thus with equal probability
$x_j \in \{N(-1, 1), N(1, 1)\}$</td></tr>
</table>

Random Forest for variable selection.

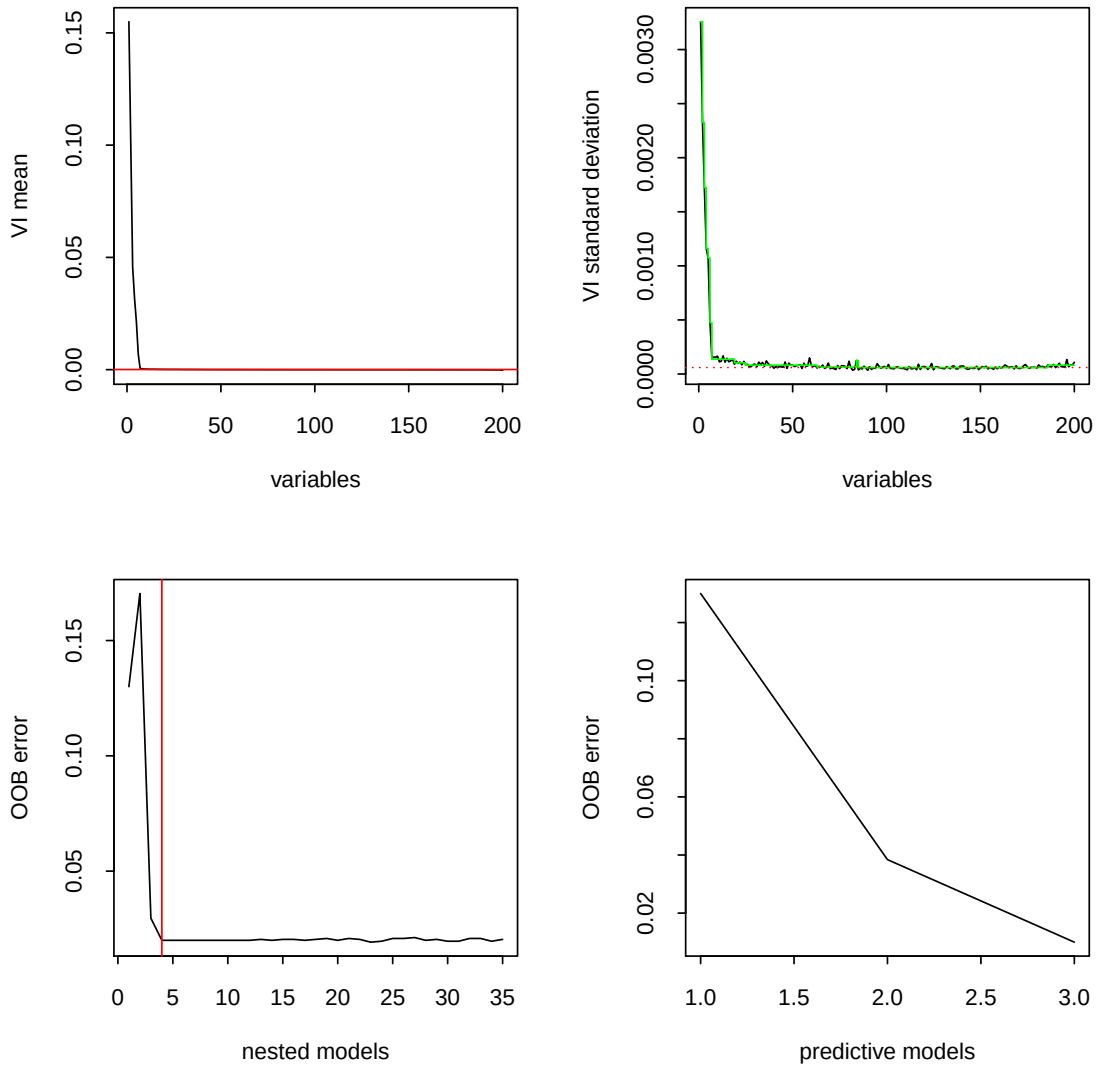
```
#
# Variable selection using Random Forests.
#   ntree=2000, number of trees.
#   mtry=number of vars. randomly sampled at each split.
toys.vsurf <- VSURF(x = toys$x, y = toys$y, mtry = 100)
names(toys.vsurf)

summary(toys.vsurf)
 VSURF computation time: 1.2 mins

 VSURF selected:
 35 variables at thresholding step (in 46.2 secs)
 4 variables at interpretation step (in 26.4 secs)
 3 variables at prediction step (in 1.3 secs)
```

Random Forest for variable selection.

```
plot(toys.vsurf)
par(opar.org)
pdf("fig_5_50_1_toys_vsurf.pdf") # Generate pdf plot.
plot(toys.vsurf)
dev.off()
(opar.org)
```

Random Forest for variable selection

VI: Variable Importance, *OOB*: Out-of-bag performance.



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