Food SR25

Food

The food data ara available at USDA's National Nutrient Database for Standard Reference [http://www.ars.usda.gov/Main/site_main.htm?modecode=12-35-45-00]. The last (2012) version is SR25.

SR25 Clamix Files

Reading the data

I selected the abbreviated data [http://www.ars.usda.gov/SP2UserFiles/Place/12354500/Data/SR25/dnload/sr25abbr.zip], downloaded them and renamed the file `abbrev.txt` to `abbrev25.txt`. Opening the file in text-editor I saw that the column 2 contains the names of foods. I tried to read the data

```
> setwd("C:/Users/Batagelj/work/clamix/clamix.R")
> a <- read.csv("./sr25/abbrev25.txt",header=FALSE,sep="^",dec=".",quote="~",row.names=2,
+  stringsAsFactors=FALSE)
Error in read.table(file = file, header = header, sep = sep, quote = quote,  :
  duplicate 'row.names' are not allowed
```

I decided to add to the end of duplicated names a string "(1)"

```
> a <- read.csv("./sr25/abbrev25.txt",header=FALSE,sep="^",dec=".",quote="~",stringsAsFactors=FALSE)
> k <- which(duplicated(a$V2))
> a$V2[k]
[1] "BABYFOOD,MEAT,BF,STR"
[2] "OIL,INDUSTRIAL,PALM KERNEL (HYDROGENATED),CONFECTION FAT"
[3] "BEEF,CHUCK,UNDER BLADE CNTR STEAK,BNLESS,DENVER CUT,LN,0\" FA"
[4] "CAMPBELL'S SEL MICROWAVEABLE BOWLS,HEA"
[5] "POPCORN,OIL-POPPED,LOFAT"
> a$V2[k] <- paste(a$V2[k],"(1)",sep="")
> a$V2[k]
[1] "BABYFOOD,MEAT,BF,STR(1)"
[2] "OIL,INDUSTRIAL,PALM KERNEL (HYDROGENATED),CONFECTION FAT(1)"
[3] "BEEF,CHUCK,UNDER BLADE CNTR STEAK,BNLESS,DENVER CUT,LN,0\" FA(1)"
[4] "CAMPBELL'S SEL MICROWAVEABLE BOWLS,HEA(1)"
[5] "POPCORN,OIL-POPPED,LOFAT(1)"
> rownames(a) <- a$V2
> rownames(a)[1:10]
 [1] "SOUP,BF BROTH OR BOUILLON,PDR,DRY"              "SOUP,BEEF BROTH,CUBED,DRY"
 [3] "SOUP,BF NOODLE,DRY,MIX"                         "SOUP,CHICK BROTH OR BOUILLON,DRY"
 [5] "SOUP,CHICK BROTH CUBES,DRY"                     "CAMPBELL'S RED & WHITE,CHICK NOODLEO'S SOUP,COND"
 [7] "CAMPBELL'S RED & WHITE,CHICK VEG SOUP,COND"     "CAMPBELL'S RED & WHITE,BF BROTH,COND"
 [9] "SOUP,ONION,DRY,MIX"                             "CAMPBELLS RED & WHITE,BF CONSOMME,COND"
```

From the documentation `SR25_doc.pdf`, pages 37-39 I obtained the list of columns / variables

```
 n  Field name    Type    Description
 1  NDB_No.       A 5*    5-digit Nutrient Databank number.
 2  Shrt_Desc     A 60    60-character abbreviated description of food item
 3  Water         N 10.2  Water (g/100 g)
 4  Energ_Kcal    N 10    Food energy (kcal/100 g)
 5  Protein       N 10.2  Protein (g/100 g)
 6  Lipid_Tot     N 10.2  Total lipid (fat)(g/100 g)
 7  Ash           N 10.2  Ash (g/100 g)
 8  Carbohydrt    N 10.2  Carbohydrate, by difference (g/100 g)
 9  Fiber_TD      N 10.1  Total dietary fiber (g/100 g)
10  Sugar_Tot     N 10.2  Total sugars (g/100 g)
11  Calcium       N 10    Calcium (mg/100 g)
12  Iron          N 10.2  Iron (mg/100 g)
13  Magnesium     N 10    Magnesium (mg/100 g)
14  Phosphorus    N 10    Phosphorus (mg/100 g)
15  Potassium     N 10    Potassium (mg/100 g)
16  Sodium        N 10    Sodium (mg/100 g)
17  Zinc          N 10.2  Zinc (mg/100 g)
18  Copper        N 10.3  Copper (mg/100 g)
19  Manganese     N 10.3  Manganese (mg/100 g)
20  Selenium      N 10.1  Selenium (µg/100 g)
21  Vit_C         N 10.1  Vitamin C (mg/100 g)
22  Thiamin       N 10.3  Thiamin (mg/100 g)
23  Riboflavin    N 10.3  Riboflavin (mg/100 g)
24  Niacin        N 10.3  Niacin (mg/100 g)
```

```
25  Panto_acid    N 10.3  Pantothenic acid (mg/100 g)
26  Vit_B6        N 10.3  Vitamin B6 (mg/100 g)
27  Folate_Tot    N 10    Folate, total (µg/100 g)
28  Folic_acid    N 10    Folic acid (µg/100 g)
29  Food_Folate   N 10    Food folate (µg/100 g)
30  Folate_DFE    N 10    Folate (µg dietary folate equivalents/100 g)
31  Choline_Tot   N 10    Choline, total (mg/100 g)
32  Vit_B12       N 10.2  Vitamin B12 (µg/100 g)
33  Vit_A_IU      N 10    Vitamin A (IU/100 g)
34  Vit_A_RAE     N 10    Vitamin A (µg retinol activity equivalents/100g)
35  Retinol       N 10    Retinol (µg/100 g)
36  Alpha_Carot   N 10    Alpha-carotene (µg/100 g)
37  Beta_Carot    N 10    Beta-carotene (µg/100 g)
38  Beta_Crypt    N 10    Beta-cryptoxanthin (µg/100 g)
39  Lycopene      N 10    Lycopene (µg/100 g)
40  Lut+Zea       N 10    Lutein+zeazanthin (µg/100 g)
41  Vit_E         N 10.2  Vitamin E (alpha-tocopherol) (mg/100 g)
42  Vit_D_mcg     N 10.1  Vitamin D (µg/100 g)
43  Vit_D_IU      N 10    Vitamin D (IU/100 g)
44  Vit_K         N 10.1  Vitamin K (phylloquinone) (µg/100 g)
45  FA_Sat        N 10.3  Saturated fatty acid (g/100 g)
46  FA_Mono       N 10.3  Monounsaturated fatty acids (g/100 g)
47  FA_Poly       N 10.3  Polyunsaturated fatty acids (g/100 g)
48  Cholestrl     N 10.3  Cholesterol (mg/100 g)
49  GmWt_1        N 9.2   First household weight for this item from the Weight file.‡
50  GmWt_Desc1    A 120   Description of household weight number 1.
51  GmWt_2        N 9.2   Second household weight for this item from the Weight file.‡
52  GmWt_Desc2    A 120   Description of household weight number 2.
53  Refuse_Pct    N 2     Percent refuse.
```

From this list we get the variable names

```
> names(a)[1:10]
 [1] "V1"  "V2"  "V3"  "V4"  "V5"  "V6"  "V7"  "V8"  "V9"  "V10"
> vn <- c(
+  "NDB_No."    , "Shrt_Desc" , "Water"     , "Energ_Kcal", "Protein"    , "Lipid_Tot"  ,
+  "Ash"        , "Carbohydrt", "Fiber_TD"  , "Sugar_Tot" , "Calcium"    , "Iron"       ,
+  "Magnesium"  , "Phosphorus", "Potassium" , "Sodium"    , "Zinc"       , "Copper"     ,
+  "Manganese"  , "Selenium"  , "Vit_C"     , "Thiamin"   , "Riboflavin" , "Niacin"     ,
+  "Panto_acid" , "Vit_B6"    , "Folate_Tot", "Folic_acid", "Food_Folate", "Folate_DFE" ,
+  "Choline_Tot", "Vit_B12"   , "Vit_A_IU"  , "Vit_A_RAE" , "Retinol"    , "Alpha_Carot",
+  "Beta_Carot" , "Beta_Crypt", "Lycopene"  , "Lut+Zea"   , "Vit_E"      , "Vit_D_mcg"  ,
+  "Vit_D_IU"   , "Vit_K"     , "FA_Sat"    , "FA_Mono"   , "FA_Poly"    , "Cholestrl"  ,
+  "GmWt_1"     , "GmWt_Desc1", "GmWt_2"    , "GmWt_Desc2", "Refuse_Pct" )
> a <- a[,-2]
> names(a) <- vn[-2]
> names(a)
 [1] "NDB_No."     "Water"       "Energ_Kcal"  "Protein"     "Lipid_Tot"   "Ash"
 [7] "Carbohydrt"  "Fiber_TD"    "Sugar_Tot"   "Calcium"     "Iron"        "Magnesium"
[13] "Phosphorus"  "Potassium"   "Sodium"      "Zinc"        "Copper"      "Manganese"
[19] "Selenium"    "Vit_C"       "Thiamin"     "Riboflavin"  "Niacin"      "Panto_acid"
[25] "Vit_B6"      "Folate_Tot"  "Folic_acid"  "Food_Folate" "Folate_DFE"  "Choline_Tot"
[31] "Vit_B12"     "Vit_A_IU"    "Vit_A_RAE"   "Retinol"     "Alpha_Carot" "Beta_Carot"
[37] "Beta_Crypt"  "Lycopene"    "Lut+Zea"     "Vit_E"       "Vit_D_mcg"   "Vit_D_IU"
[43] "Vit_K"       "FA_Sat"      "FA_Mono"     "FA_Poly"     "Cholestrl"   "GmWt_1"
[49] "GmWt_Desc1"  "GmWt_2"      "GmWt_Desc2"  "Refuse_Pct"
> dim(a)
[1] 8194   52
> food <- a
> save(food,file="./sr25/sr25.Rdata")
```

I removed the second variable (food name) from the data frame and replaced the variable names with the names from the list. I have finally the data in the form of the R data frame. I save it on the file `sr25.Rdata` .

Encoding the data

I suppose that the encoding rules `encFood.R` for SR22 can be useful also for SR25. I copied them to the sr25 directory.

```
encWater <- list(
  "[0]"           = function(x) x<=0,
  "(0,5.65]"      = function(x) x<=5.65,
  "(5.65,29.5]"   = function(x) x<=29.5,
  "(29.5,53.9)"   = function(x) x< 53.9,
  "[53.9,62.4)"   = function(x) x< 62.4,
  "[62.4,70.75)"  = function(x) x< 70.75,
  "[70.75,78.05]" = function(x) x<=78.05,
```

```
  "(78.05,88)"    = function(x) x< 88,
  "[88,100]"      = function(x) x<=100,
  "NA"            = function(x) TRUE )

encEnergKC <- list(
  "[0]"           = function(x) x<=0,
  "(0,50]"        = function(x) x<=50,
  "(50,104]"      = function(x) x<=104,
  "(104,160]"     = function(x) x<=160,
  "(160,232]"     = function(x) x<=232,
  "(232,312]"     = function(x) x<=312,
  "(312,386]"     = function(x) x<=386,
  "(386,800)"     = function(x) x< 800,
  "[800,905]"     = function(x) x<=905,
  "NA"            = function(x) TRUE )

encProtein <- list(
  "[0]"           = function(x) x<=0,
  "(0,1.5]"       = function(x) x<=1.5,
  "(1.5,4.1]"     = function(x) x<=4.1,
  "(4.1,8.4)"     = function(x) x< 8.4,
  "[8.4,16]"      = function(x) x<=16,
  "(16,23.05)"    = function(x) x< 23.05,
  "[23.05,37]"    = function(x) x<=37,
  "(37,75)"       = function(x) x< 75,
  "[75,90]"       = function(x) x<=90,
  "NA"            = function(x) TRUE )

encTotLipi <- list(
  "[0]"           = function(x) x<=0,
  "(0,0.3]"       = function(x) x<=0.3,
  "(0.3,1.3)"     = function(x) x< 1.3,
  "[1.3,3.8)"     = function(x) x< 3.8,
  "[3.8,8)"       = function(x) x< 8,
  "[8,13.7)"      = function(x) x< 13.7,
  "[13.7,23.5)"   = function(x) x< 23.5,
  "[23.5,85)"     = function(x) x< 85,
  "[85,100]"      = function(x) x<=100,
  "NA"            = function(x) TRUE )

encAsh <- list(
  "[0]"           = function(x) x<=0,
  "(0,0.7)"       = function(x) x< 0.7,
  "[0.7,1)"       = function(x) x< 1,
  "[1,1.24)"      = function(x) x< 1.24,
  "[1.24,1.75)"   = function(x) x< 1.75,
  "[1.75,3)"      = function(x) x< 3,
  "[3,45)"        = function(x) x< 45,
  "[45,95)"       = function(x) x< 95,
  "[95,100]"      = function(x) x<=100,
  "NA"            = function(x) TRUE )

encCarbohyd <- list(
  "[0]"           = function(x) x<=0,
  "(0,3.5]"       = function(x) x<=3.5,
  "(3.5,6.85]"    = function(x) x<=6.85,
  "(6.85,11.35]"  = function(x) x<=11.35,
  "(11.35,18.1)"  = function(x) x< 18.1,
  "[18.1,27.8]"   = function(x) x<=27.8,
  "(27.8,55.1]"   = function(x) x<=55.1,
  "(55.1,73]"     = function(x) x<=73,
  "(73,100]"      = function(x) x<=100,
  "NA"            = function(x) TRUE )

encFiberTd <- list(
  "[0]"           = function(x) x<=0,
  "(0,0.8]"       = function(x) x<=0.8,
  "(0.8,1.5]"     = function(x) x<=1.5,
  "(1.5,2.1]"     = function(x) x<=2.1,
  "(2.1,3.1]"     = function(x) x<=3.1,
  "(3.1,5.6]"     = function(x) x<=5.6,
  "(5.6,35]"      = function(x) x<=35,
  "(35,60]"       = function(x) x<=60,
  "(60,90]"       = function(x) x<=90,
  "NA"            = function(x) TRUE )

encCalcium <- list(
  "[0]"           = function(x) x<=0,
  "(0,7]"         = function(x) x<=7,
  "(7,12]"        = function(x) x<=12,
  "(12,20]"       = function(x) x<=20,
  "(20,34]"       = function(x) x<=34,
  "(34,69]"       = function(x) x<=69,
  "(69,159]"      = function(x) x<=159,
  "(159,3000]"    = function(x) x<=3000,
  "(3000,7400]"   = function(x) x<=7400,
```

```
  "NA"            = function(x) TRUE )

encIron <- list(
  "[0]"           = function(x) x<=0,
  "(0,0.35]"      = function(x) x<=0.35,
  "(0.35,0.75]"   = function(x) x<=0.75,
  "(0.75,1.2]"    = function(x) x<=1.2,
  "(1.2,1.8]"     = function(x) x<=1.8,
  "(1.8,2.5]"     = function(x) x<=2.5,
  "(2.5,3.85]"    = function(x) x<=3.85,
  "(3.85,80]"     = function(x) x<=80,
  "(80,125]"      = function(x) x<=125,
  "NA"            = function(x) TRUE )

encMagnesiu <- list(
  "[0]"           = function(x) x<=0,
  "(0,9)"         = function(x) x< 9,
  "[9,16)"        = function(x) x< 16,
  "[16,21)"       = function(x) x< 21,
  "[21,25)"       = function(x) x< 25,
  "[25,32)"       = function(x) x< 32,
  "[32,65)"       = function(x) x< 65,
  "[65,600)"      = function(x) x< 600,
  "[600,900]"     = function(x) x<=900,
  "NA"            = function(x) TRUE )

encPhosphor <- list(
  "[0]"           = function(x) x<=0,
  "(0,25)"        = function(x) x< 25,
  "[25,60)"       = function(x) x< 60,
  "[60,112)"      = function(x) x< 112,
  "[112,172)"     = function(x) x< 172,
  "[172,208)"     = function(x) x< 208,
  "[208,268)"     = function(x) x< 268,
  "[268,6000)"    = function(x) x< 6000,
  "[6000,10000]"  = function(x) x<=10000,
  "NA"            = function(x) TRUE )

encPotassium <- list(
  "[0]"           = function(x) x<=0,
  "(0,90)"        = function(x) x< 90,
  "[90,147)"      = function(x) x< 147,
  "[147,211)"     = function(x) x< 211,
  "[211,281)"     = function(x) x< 281,
  "[281,340)"     = function(x) x< 340,
  "[340,426)"     = function(x) x< 426,
  "[426,6000)"    = function(x) x< 6000,
  "[6000,17000]"  = function(x) x<=17000,
  "NA"            = function(x) TRUE )

encSodium <- list(
  "[0]"           = function(x) x<=0,
  "(0,10)"        = function(x) x< 10,
  "[10,50)"       = function(x) x< 50,
  "[50,66)"       = function(x) x< 66,
  "[66,121)"      = function(x) x< 121,
  "[121,351)"     = function(x) x< 351,
  "[351,655)"     = function(x) x< 655,
  "[655,15000)"   = function(x) x< 15000,
  "[15000,30000]" = function(x) x<=30000,
  "NA"            = function(x) TRUE )

encZinc <- list(
  "[0]"           = function(x) x<=0,
  "(0,0.23)"      = function(x) x< 0.23,
  "[0.23,0.53)"   = function(x) x< 0.53,
  "[0.53,1.06)"   = function(x) x< 1.06,
  "[1.06,2.23)"   = function(x) x< 2.23,
  "[2.23,4.12)"   = function(x) x< 4.12,
  "[4.12,20)"     = function(x) x< 20,
  "[20,150)"      = function(x) x< 150,
  "[150,200]"     = function(x) x<=200,
  "NA"            = function(x) TRUE )

encCopper <- list(
  "[0]"           = function(x) x<=0,
  "(0,0.045)"     = function(x) x< 0.045,
  "[0.045,0.071)" = function(x) x< 0.071,
  "[0.071,0.1)"   = function(x) x< 0.1,
  "[0.1,0.135)"   = function(x) x< 0.135,
  "[0.135,0.23)"  = function(x) x< 0.23,
  "[0.23,0.95)"   = function(x) x< 0.95,
  "[0.95,6.5)"    = function(x) x< 6.5,
  "[6.5,10]"      = function(x) x<=10,
  "NA"            = function(x) TRUE )
```

```
encManganes <- list(
  "[0]"           = function(x) x<=0,
  "(0,0.016)"     = function(x) x< 0.016,
  "[0.016,0.028)" = function(x) x< 0.028,
  "[0.028,0.118)" = function(x) x< 0.118,
  "[0.118,0.27)"  = function(x) x< 0.27,
  "[0.27,0.71)"   = function(x) x< 0.71,
  "[0.71,10)"     = function(x) x< 10,
  "[10,70)"       = function(x) x< 70,
  "[70,80]"       = function(x) x<=80,
  "NA"            = function(x) TRUE )

encSelenium <- list(
  "[0]"           = function(x) x<=0,
  "(0,0.8)"       = function(x) x< 0.8,
  "[0.8,3)"       = function(x) x< 3,
  "[3,11]"        = function(x) x<=11,
  "(11,20)"       = function(x) x< 20,
  "[20,28.5)"     = function(x) x< 28.5,
  "[28.5,160)"    = function(x) x< 160,
  "[160,1500)"    = function(x) x< 1500,
  "[1500,3000]"   = function(x) x<=3000,
  "NA"            = function(x) TRUE )

encVitA <- list(
  "[0]"           = function(x) x<=0,
  "(0,15]"        = function(x) x<=15,
  "(15,52]"       = function(x) x<=52,
  "(52,118]"      = function(x) x<=118,
  "(118,230]"     = function(x) x<=230,
  "(230,560]"     = function(x) x<=560,
  "(560,1800]"    = function(x) x<=1800,
  "(1800,50000]"  = function(x) x<=50000,
  "(50000,100000]"= function(x) x<=100000,
  "NA"            = function(x) TRUE )

encVitE <- list(
  "[0]"           = function(x) x<=0,
  "(0,0.13)"      = function(x) x< 0.13,
  "[0.13,0.2]"    = function(x) x<=0.2,
  "(0.2,0.3]"     = function(x) x<=0.3,
  "(0.3,0.63]"    = function(x) x<=0.63,
  "(0.63,1.5]"    = function(x) x<=1.5,
  "(1.5,20)"      = function(x) x< 20,
  "[20,190]"      = function(x) x<=190,
  "(190,195]"     = function(x) x<=195,
  "NA"            = function(x) TRUE )

encVitC  <- list(
  "[0]"           = function(x) x<=0,
  "(0,0.5)"       = function(x) x< 0.5,
  "[0.5,1]"       = function(x) x<=1,
  "(1,2.5)"       = function(x) x< 2.5,
  "[2.5,6)"       = function(x) x< 6,
  "[6,13.5)"      = function(x) x< 13.5,
  "[13.5,34)"     = function(x) x< 34,
  "[34,1500)"     = function(x) x< 1500,
  "[1500,2400]"   = function(x) x<=2400,
  "NA"            = function(x) TRUE )

encThiamin  <- list(
  "[0]"           = function(x) x<=0,
  "(0,0.025]"     = function(x) x<=0.025,
  "(0.025,0.05]"  = function(x) x<=0.05,
  "(0.05,0.08)"   = function(x) x<=0.08,
  "[0.08,0.105]"  = function(x) x<=0.105,
  "(0.105,0.19)"  = function(x) x< 0.19,
  "[0.19,0.42)"   = function(x) x< 0.42,
  "[0.42,8)"      = function(x) x< 8,
  "[8,15]"        = function(x) x<=15,
  "NA"            = function(x) TRUE )

encRibolfla  <- list(
  "[0]"           = function(x) x<=0,
  "(0,0.036]"     = function(x) x<=0.036,
  "(0.036,0.076]" = function(x) x<=0.076,
  "(0.076,0.14)"  = function(x) x< 0.14,
  "[0.14,0.192)"  = function(x) x< 0.192,
  "[0.192,0.25]"  = function(x) x<=0.25,
  "(0.25,0.36]"   = function(x) x<=0.36,
  "(0.36,5]"      = function(x) x<=5,
  "(5,7]"         = function(x) x<=7,
  "NA"            = function(x) TRUE )

encNiacin  <- list(
  "[0]"           = function(x) x<=0,
```

```
  "(0,0.35]"      = function(x) x<=0.35,
  "(0.35,0.93)"   = function(x) x< 0.93,
  "[0.93,2.26)"   = function(x) x< 2.26,
  "[2.26,3.75]"   = function(x) x<=3.75,
  "(3.75,5.41]"   = function(x) x<=5.41,
  "(5.41,25]"     = function(x) x<=25,
  "(25,60)"       = function(x) x< 60,
  "[60,80]"       = function(x) x<=80,
  "NA"            = function(x) TRUE )

encPantoAc <- list(
  "[0]"           = function(x) x<=0,
  "(0,0.125)"     = function(x) x< 0.125,
  "[0.125,0.27)"  = function(x) x< 0.27,
  "[0.27,0.36]"   = function(x) x<=0.36,
  "(0.36,0.53]"   = function(x) x<=0.53,
  "(0.53,0.83)"   = function(x) x< 0.83,
  "[0.83,15)"     = function(x) x< 15,
  "[15,30)"       = function(x) x< 30,
  "[30,40]"       = function(x) x<=40,
  "NA"            = function(x) TRUE )

encVitB6 <- list(
  "[0]"           = function(x) x<=0,
  "(0,0.037]"     = function(x) x<=0.037,
  "(0.037,0.07]"  = function(x) x<=0.07,
  "(0.07,0.12]"   = function(x) x<=0.12,
  "(0.12,0.215]"  = function(x) x<=0.215,
  "(0.215,0.33]"  = function(x) x<=0.33,
  "(0.33,0.43]"   = function(x) x<=0.43,
  "(0.43,5)"      = function(x) x< 5,
  "[5,8]"         = function(x) x<=8,
  "NA"            = function(x) TRUE )

encFolate <- list(
  "[0]"           = function(x) x<=0,
  "(0,5)"         = function(x) x< 5,
  "[5,8)"         = function(x) x< 8,
  "[8,12)"        = function(x) x< 12,
  "[12,23)"       = function(x) x< 23,
  "[23,48)"       = function(x) x< 48,
  "[48,115)"      = function(x) x< 115,
  "[115,1000)"    = function(x) x< 1000,
  "[1000,2350]"   = function(x) x<=2350,
  "NA"            = function(x) TRUE )

encVitB12  <- list(
  "[0]"           = function(x) x<=0,
  "(0,0.12]"      = function(x) x<=0.12,
  "(0.12,0.3]"    = function(x) x<=0.3,
  "(0.3,0.6]"     = function(x) x<=0.6,
  "(0.6,1.4]"     = function(x) x<=1.4,
  "(1.4,2.47]"    = function(x) x<=2.47,
  "(2.47,3)"      = function(x) x< 3,
  "[3,60)"        = function(x) x< 60,
  "[60,120]"      = function(x) x<=120,
  "NA"            = function(x) TRUE )

encFaSat  <- list(
  "[0]"           = function(x) x<=0,
  "(0,0.054)"     = function(x) x< 0.054,
  "[0.054,0.29)"  = function(x) x< 0.29,
  "[0.29,1.08)"   = function(x) x< 1.08,
  "[1.08,2.4)"    = function(x) x< 2.4,
  "[2.4,4.3]"     = function(x) x<=4.3,
  "(4.3,7.9]"     = function(x) x<=7.9,
  "(7.9,80)"      = function(x) x< 80,
  "[80,100]"      = function(x) x<=100,
  "NA"            = function(x) TRUE )

encFaMono  <- list(
  "[0]"           = function(x) x<=0,
  "(0,0.035]"     = function(x) x<=0.035,
  "(0.035,0.3]"   = function(x) x<=0.3,
  "(0.3,1.25)"    = function(x) x< 1.25,
  "[1.25,3]"      = function(x) x<=3,
  "(3,5.6)"       = function(x) x< 5.6,
  "[5.6,9.5)"     = function(x) x< 9.5,
  "[9.5,65)"      = function(x) x< 65,
  "[65,85]"       = function(x) x<=85,
  "NA"            = function(x) TRUE )

encFaPoly  <- list(
  "[0]"           = function(x) x<=0,
  "(0,0.115]"     = function(x) x<=0.115,
  "(0.115,0.335]" = function(x) x<=0.335,
```

```
  "(0.335,0.685]" = function(x) x<=0.685,
  "(0.685,1.23)"  = function(x) x< 1.23,
  "[1.23,2.73)"   = function(x) x< 2.73,
  "[2.73,40)"     = function(x) x< 40,
  "[40,60)"       = function(x) x< 60,
  "[60,75]"       = function(x) x<=75,
  "NA"            = function(x) TRUE )

encCholestr  <- list(
  "[0]"           = function(x) x<=0,
  "(0,12]"        = function(x) x<=12,
  "(12,45]"       = function(x) x<=45,
  "(45,66]"       = function(x) x<=66,
  "(66,80]"       = function(x) x<=80,
  "(80,94]"       = function(x) x<=94,
  "(94,550]"      = function(x) x<=550,
  "(550,1900]"    = function(x) x<=1900,
  "(1900,3100]"   = function(x) x<=3100,
  "NA"            = function(x) TRUE )
```

May be we can include into analysis some additional variables. Then we need to add also the encoding rules for them.

Here is the list of variables and corresponding rules

```
 1  NDB_No.
 2  Water          encWater
 3  Energ_Kcal     encEnergKC
 4  Protein        encProtein
 5  Lipid_Tot      encTotLipi
 6  Ash            encAsh
 7  Carbohydrt     encCarbohyd
 8  Fiber_TD       encFiberTd
 9  Sugar_Tot
10  Calcium        encCalcium
11  Iron           encIron
12  Magnesium      encMagnesiu
13  Phosphorus     encPhosphor
14  Potassium      encPotassium
15  Sodium         encSodium
16  Zinc           encZinc
17  Copper         encCopper
18  Manganese      encManganes
19  Selenium       encSelenium
20  Vit_C          encVitC
21  Thiamin        encThiamin
22  Riboflavin     encRibolfla
23  Niacin         encNiacin
24  Panto_acid     encPantoAc
25  Vit_B6         encVitB6
26  Folate_Tot
27  Folic_acid
28  Food_Folate
29  Folate_DFE
30  Choline_Tot
31  Vit_B12        encVitB12
32  Vit_A_IU
33  Vit_A_RAE
34  Retinol
35  Alpha_Carot
36  Beta_Carot
37  Beta_Crypt
38  Lycopene
39  Lut+Zea
40  Vit_E          encVitE
41  Vit_D_mcg
42  Vit_D_IU
43  Vit_K
44  FA_Sat         encFaSat
45  FA_Mono        encFaMono
46  FA_Poly        encFaPoly
47  Cholestrl      encCholestr
48  GmWt_1
49  GmWt_Desc1
50  GmWt_2
51  GmWt_Desc2
52  Refuse_Pct
                   encVitA
                   encFolate
```

Now we can read the data in R, select the variables to be transformed and match them with the corresponding encoding rules - prepare the vectors `s` and `enc`.

```
> setwd("C:/Users/Batagelj/work/clamix/clamix.R")
> load("./sr25/sr25.Rdata")
> (numSO <- nrow(food))
[1] 8194
> source("C:\\Users\\Batagelj\\work\\clamix\\clamix.R\\clamix3.R")
> source("C:\\Users\\Batagelj\\work\\clamix\\clamix.R\\sr25\\encFood.R")
> (s <- c(2:8,10:25,31,40,44:47))
 [1]  2  3  4  5  6  7  8 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 31 40
[26] 44 45 46 47
> nVar <- length(s)
> enc <- c("encWater",  "encEnergKC", "encProtein", "encTotLipi", "encAsh",
+   "encCarbohyd", "encFiberTd", "encCalcium", "encIron", "encMagnesiu",
+   "encPhosphor", "encPotassium", "encSodium", "encZinc", "encCopper",
+   "encManganes", "encSelenium", "encVitC", "encThiamin", "encRibolfla",
+   "encNiacin", "encPantoAc", "encVitB6", "encVitB12", "encVitE",
+   "encFaSat", "encFaMono", "encFaPoly", "encCholestr" )
>
> for(i in 1:nVar) cat(i,s[i],names(food)[s[i]]," > ",enc[i],'\n')
1 2 Water  >  encWater
2 3 Energ_Kcal  >  encEnergKC
3 4 Protein  >  encProtein
4 5 Lipid_Tot  >  encTotLipi
5 6 Ash  >  encAsh
6 7 Carbohydrt  >  encCarbohyd
7 8 Fiber_TD  >  encFiberTd
8 10 Calcium  >  encCalcium
9 11 Iron  >  encIron
10 12 Magnesium  >  encMagnesiu
11 13 Phosphorus  >  encPhosphor
12 14 Potassium  >  encPotassium
13 15 Sodium  >  encSodium
14 16 Zinc  >  encZinc
15 17 Copper  >  encCopper
16 18 Manganese  >  encManganes
17 19 Selenium  >  encSelenium
18 20 Vit_C  >  encVitC
19 21 Thiamin  >  encThiamin
20 22 Riboflavin  >  encRibolfla
21 23 Niacin  >  encNiacin
22 24 Panto_acid  >  encPantoAc
23 25 Vit_B6  >  encVitB6
24 31 Vit_B12  >  encVitB12
25 40 Vit_E  >  encVitE
26 44 FA_Sat  >  encFaSat
27 45 FA_Mono  >  encFaMono
28 46 FA_Poly  >  encFaPoly
29 47 Cholestrl  >  encCholestr
```

The variables and rules match.

Now we are ready to encode all selected variables.

```
foodSO <- vector("list",nVar)
for(i in 1:nVar){
  var <- food[[s[[i]]]]
  foodSO[[i]] <- sapply(var,function(x) encodeSO(x,get(enc[[i]]),10))
  names(foodSO)[[i]] <- names(food)[[s[[i]]]]
}
```

Let us prepare also the metadata. First the names of categories for each variable.

```
> nVarP <- nVar+1
> varCats <- vector("list",nVar)
> varCats[[1]]  <- names(encWater)
> varCats[[2]]  <- names(encEnergKC)
> varCats[[3]]  <- names(encProtein)
> varCats[[4]]  <- names(encTotLipi)
> varCats[[5]]  <- names(encAsh)
> varCats[[6]]  <- names(encCarbohyd)
> varCats[[7]]  <- names(encFiberTd)
> varCats[[8]]  <- names(encCalcium)
> varCats[[9]]  <- names(encIron)
> varCats[[10]] <- names(encMagnesiu)
> varCats[[11]] <- names(encPhosphor)
> varCats[[12]] <- names(encPotassium)
> varCats[[13]] <- names(encSodium)
> varCats[[14]] <- names(encZinc)
> varCats[[15]] <- names(encCopper)
> varCats[[16]] <- names(encManganes)
> varCats[[17]] <- names(encSelenium)
> varCats[[18]] <- names(encVitC)
> varCats[[19]] <- names(encThiamin)
```

```
> varCats[[20]] <- names(encRibolfla)
> varCats[[21]] <- names(encNiacin)
> varCats[[22]] <- names(encPantoAc)
> varCats[[23]] <- names(encVitB6)
> varCats[[24]] <- names(encVitB12)
> varCats[[25]] <- names(encVitE)
> varCats[[26]] <- names(encFaSat)
> varCats[[27]] <- names(encFaMono)
> varCats[[28]] <- names(encFaPoly)
> varCats[[29]] <- names(encCholestr)
>
> varCats[[15]]
 [1] "[0]"           "(0,0.045)"     "[0.045,0.071)" "[0.071,0.1)"
 [5] "[0.1,0.135)"   "[0.135,0.23)"  "[0.23,0.95)"   "[0.95,6.5)"
 [9] "[6.5,10]"      "NA"
> nCats <- sapply(varCats,length)
> names(varCats) <- names(foodSO)
```

Let us create the empty symbolic object `so` and symbolic object `namedSO` with named components and save the metadata.

```
> long <- rownames(food)
> so <- emptySO(nCats)
> namedSO <- so
> names(namedSO) <- names(varCats)
> for(i in 1:nVar) varCats[[i]] <- c(varCats[[i]],"num")
> for(i in 1:nVar) names(namedSO[[i]]) <- varCats[[i]]
> save(nVar,nVarP,so,namedSO,numSO,long,varCats,file="./sr25/sr25.meta")
```

Finally we transform the recoded data into symbolic objects describing single units and save them.

```
> SOs <- vector("list",numSO)
> for(i in 1:numSO){
+   st <- so
+   for(j in 1:nVar)
+     {st[[j]][foodSO[[j]][[i]]] <- 1; st[[j]][[nCats[[j]]+1]] <- 1}
+ #  names(SOs)[[i]] <- long[[i]]
+   SOs[[i]] <- st
+ }
> save(nVar,nVarP,so,numSO,SOs,file="./sr25/sr25.so")
```

Basic quantities

- `nVar` - number of variables
- `nVarP = nVar+1`
- `long` - names of units
- `SOs` - set of units represented as symbolic objects
- `numSO` - number of symbolic objects (units)
- `varCats` - list with names variables and names of categories for each variable
- `nCats` - number of categories for each variable
- `so` - empty symbolic object
- `namedSO` - empty symbolic object with named components

The main idea is that all computations are done on SOs without named components (to reduce the work) and to use names only in the presentation of results.

Automatic encoding

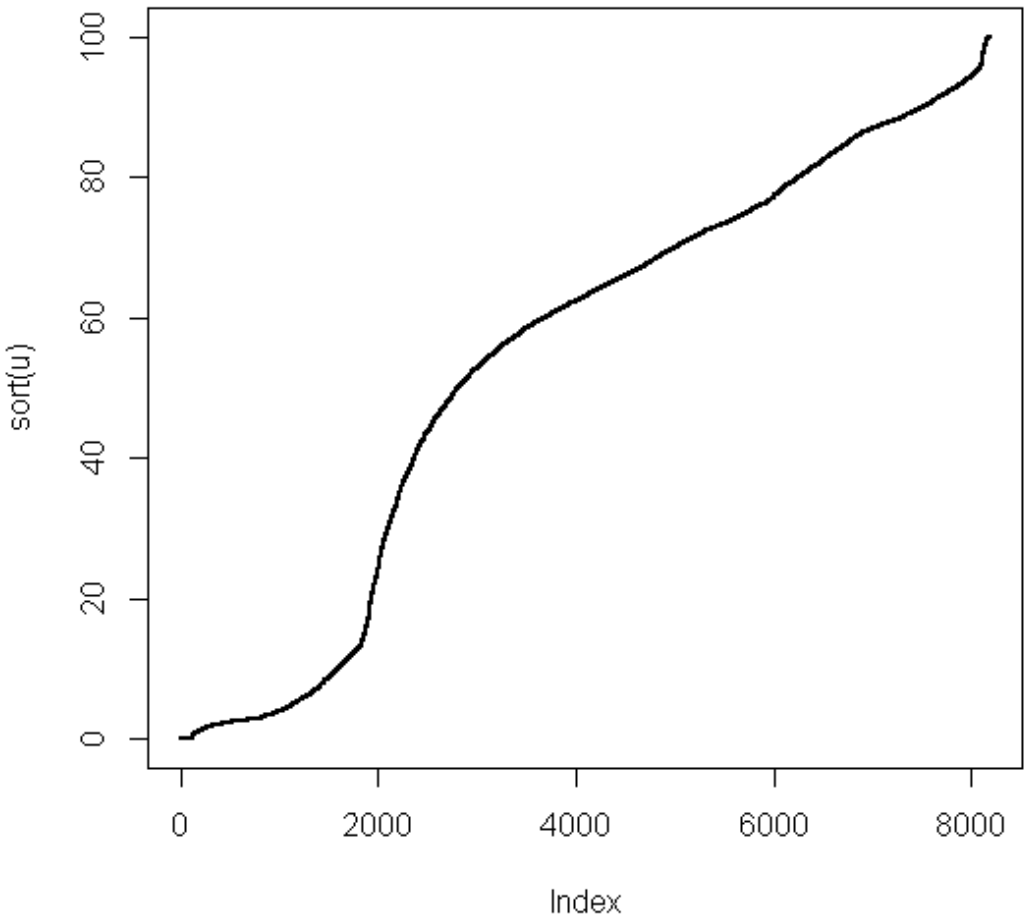
An approach to determine the encoding rules for a numerical variable is to select the number of categories (bins) and then determine the breaks so that each category gets approximately the same number of units.

Water

For example, for a variable water into 10 categories:

```
> v <- food$Water
> u <- v[!is.na(v)]
```

```
> plot(sort(u),pch=20,cex=0.5)
```



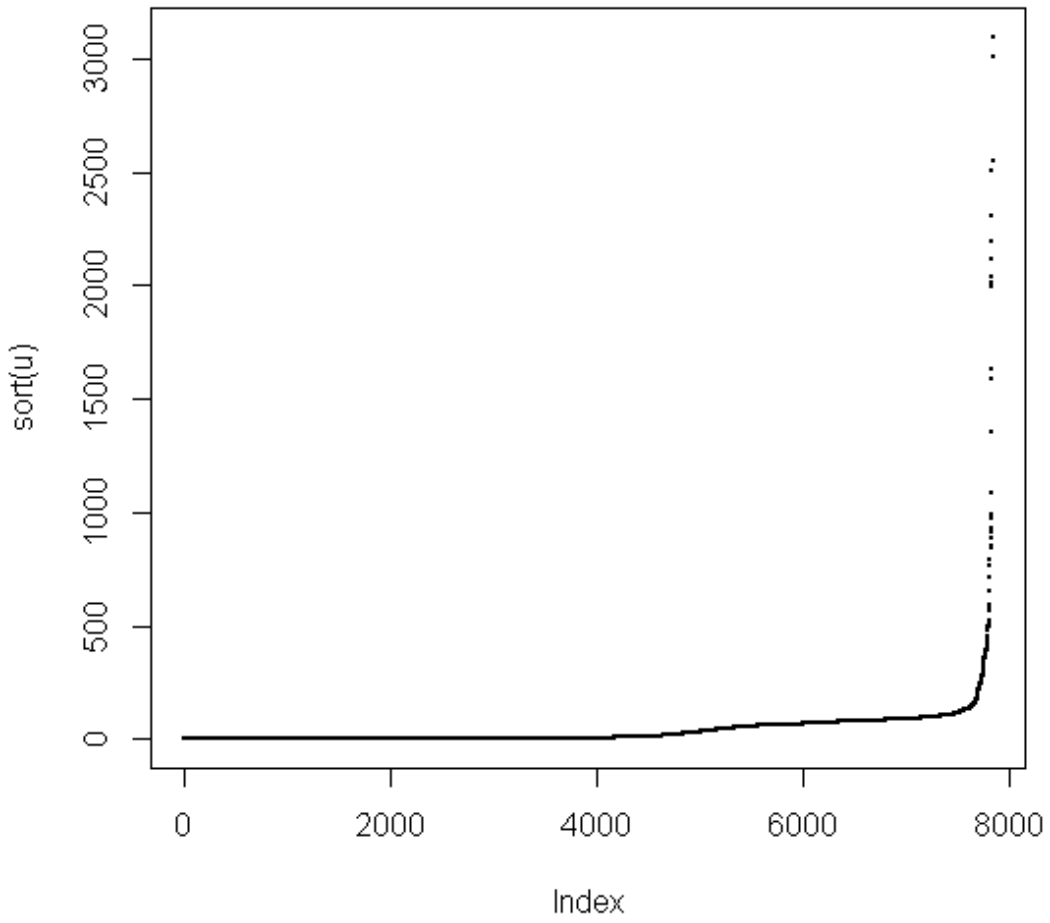
The picture doesn't show any special irregularities. We can proceed with encoding

```
> (brks <- quantile(u, seq(0,1,1/10)))
     0%     10%     20%     30%     40%     50%     60%     70%     80%     90%
  0.000   3.000  10.504  42.621  56.138  62.980  69.202  74.860  82.836  88.910
   100%
100.000
> r <- findInterval(v,brks)
> table(r)
r
  1   2   3   4   5   6   7   8   9  10  11
732 906 819 818 818 820 817 820 818 816   4
> r[r==11] <- 10
> (T <- c(as.vector(table(r)),length(r[is.na(r)])))
 [1] 732 906 819 818 818 820 817 820 818 820   6
```

At the end of table we append the number of NA values.

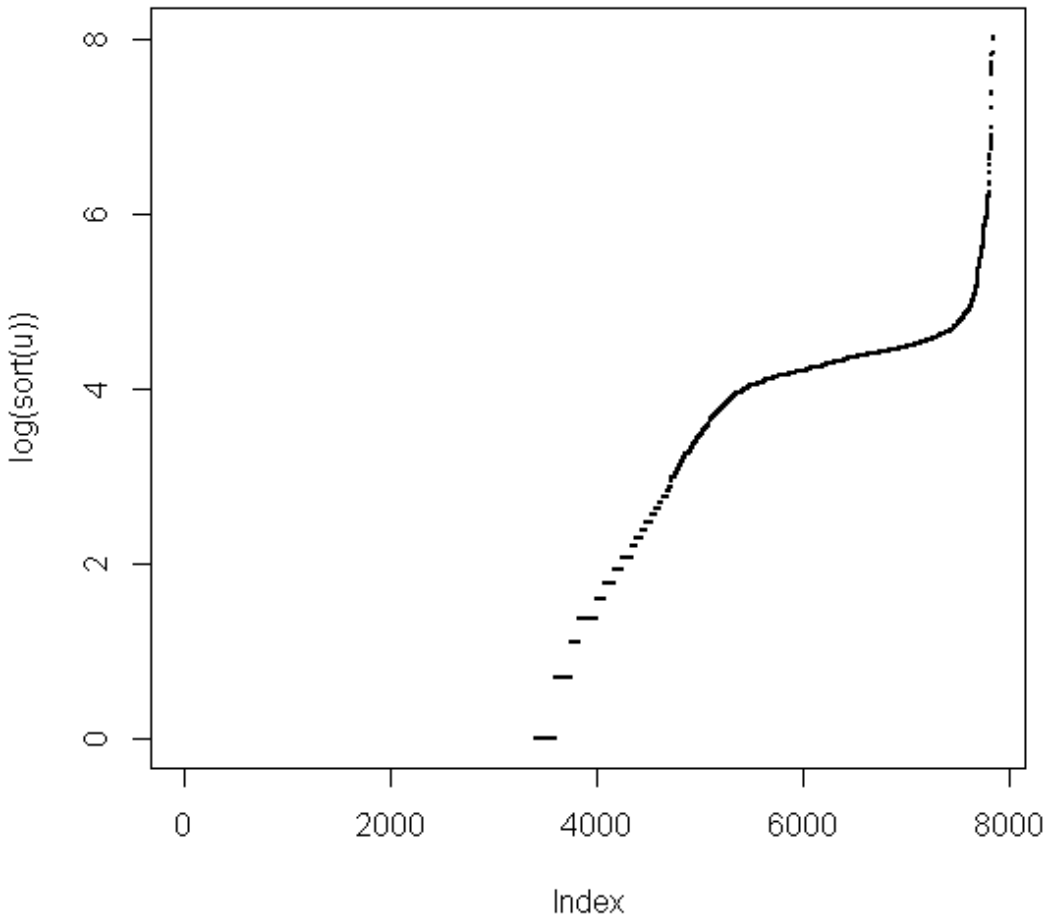
Cholesterol

```
> v <- food$Cholestrl
> u <- v[!is.na(v)]
> plot(sort(u),pch=20,cex=0.5)
```



The range of variable's values is large. We'll get a better picture in log-scale

```
> plot(log(sort(u)),pch=20,cex=0.5)
```

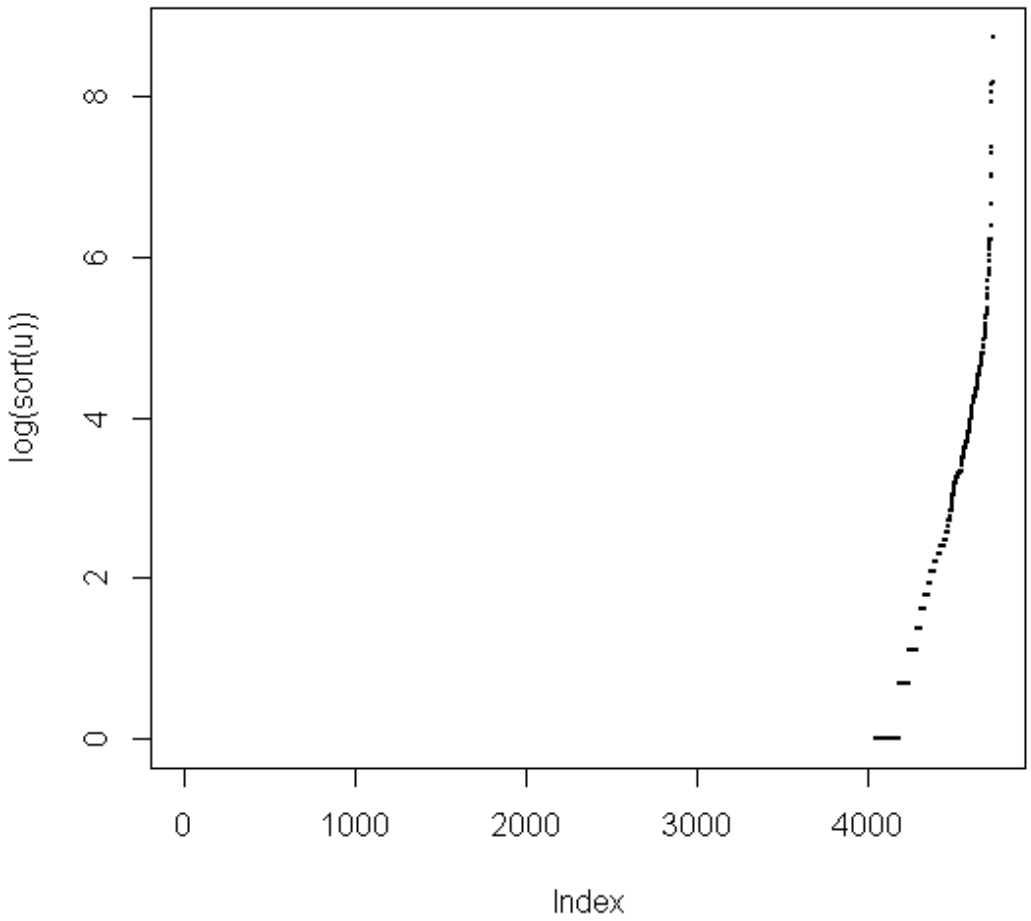


we see that there are many zero values. We determine the breaks on the positive values and then combine them with zeros and NAs.

```
> (brks <- quantile(u[u>0], seq(0,1,1/9)))
       0% 11.11111% 22.22222% 33.33333% 44.44444% 55.55556% 66.66667% 77.77778%
        1         4        10        27        53        66        76        86
88.88889%      100%
      102      3100
> r <- findInterval(v,brks)
> r[r==10] <- 9
> (T <- c(as.vector(table(r)),length(r[is.na(r)])))
 [1] 3413  415  554  503  486  491  483  494  488  507  360
```

Beta-cryptoxanthin

```
> v <- food$Beta_Crypt
> u <- v[!is.na(v)]
> plot(log(sort(u)),pch=20,cex=0.5)
```



From the picture we see that there are many zero and many NA values. We proceed similary as in the case of Cholesterol.

```
> (brks <- quantile(u[u>0], seq(0,1,1/10)))
    0%    10%    20%    30%    40%    50%    60%    70%    80%    90%   100%
   1.0    1.0    1.0    3.0    5.0    8.0   12.0   26.0   47.0  108.6 6252.0
> bs <- c(1,2,as.vector(brks)[4:11])
> bs
 [1]    1.0    2.0    3.0    5.0    8.0   12.0   26.0   47.0  108.6 6252.0
> r <- findInterval(v,bs)
> table(r)
r
   0    1    2    3    4    5    6    7    8    9   10
4039  144   61   62   65   80   67   73   70   69    1
> r[r==10] <- 9
> table(r)
r
   0    1    2    3    4    5    6    7    8    9
4039  144   61   62   65   80   67   73   70   70
> (T <- c(as.vector(table(r)),length(r[is.na(r)])))
 [1] 4039  144   61   62   65   80   67   73   70   70 3463
> names(T) <- c("<1","<2",paste("<",as.character(brks)[4:10],sep=""),
+   paste("<=",as.character(brks)[11],sep=""),"NA")
> T
    <1     <2     <3     <5     <8    <12    <26    <47 <108.6 <=6252     NA
  4039    144     61     62     65     80     67     73     70     70   3463
> length(v[!is.na(v)&(12<=v)&(v<26)])
[1] 67
> a <- c("0","1","2",as.character(brks)[4:11])
> names(T) <- c(paste("[",a[1:9],",",a[2:10],")",sep=""),
+   paste("[",a[10],",",a[11],"]",sep=""))
> T
       [0,1)        [1,2)        [2,3)        [3,5)        [5,8)       [8,12)
        4039          144           61           62           65           80
    [12,26)      [26,47)   [47,108.6) [108.6,6252]         <NA>
          67           73           70           70         3463
```

Folic acid

```
> v <- food$Folic_acid
> u <- v[!is.na(v)]
> plot(log(sort(u)),pch=20,cex=0.5)
> (brks <- quantile(u[u>0], seq(0,1,1/9)))
       0% 11.11111% 22.22222% 33.33333% 44.44444% 55.55556% 66.66667% 77.77778%
   1.0000    9.0000   17.0000   25.0000   38.0000   54.0000   77.0000  140.0000
88.88889%      100%
 328.6667 3269.0000
> r <- findInterval(v,brks)
> table(r)
r
   0    1    2    3    4    5    6    7    8    9   10
5273  112  133  120  127  126  126  124  125  124    1
> r[r==10] <- 9
> a <- c("0",as.character(brks))
> (T <- c(as.vector(table(r)),length(r[is.na(r)])))
 [1] 5273  112  133  120  127  126  126  124  125  125 1803
> names(T) <- c(paste("[",a[1:10],",",a[2:11],")",sep=""),"NA")
> T
                  [0,1)                   [1,9)                  [9,17)
                   5273                     112                     133
                [17,25)                 [25,38)                 [38,54)
                    120                     127                     126
                [54,77)                [77,140)  [140,328.666666666666)
                    126                     124                     125
[328.666666666666,3269)                      NA
                    125                    1803
```

Analysis

Now we are ready for analysis. First we determine using leaders method 25 leaders. We cluster them further using the hierarchical method and plot the dendrogram.

```
setwd("C:/Users/Batagelj/work/clamix/clamix.R")
source("C:\\Users\\Batagelj\\work\\clamix\\clamix.R\\clamix3.R")
load("./sr25/sr25.so")
load("./sr25/sr25.meta")
alpha <-rep(1/nVar,nVar)
rez <- leaderSO(SOs,25)
save(rez,file="./sr25/sr25.rez")
hc <- hclustSO(rez$leaders)
plot(hc,hang=-1)
long[rez$clust==9]
long[rez$clust==1]
```

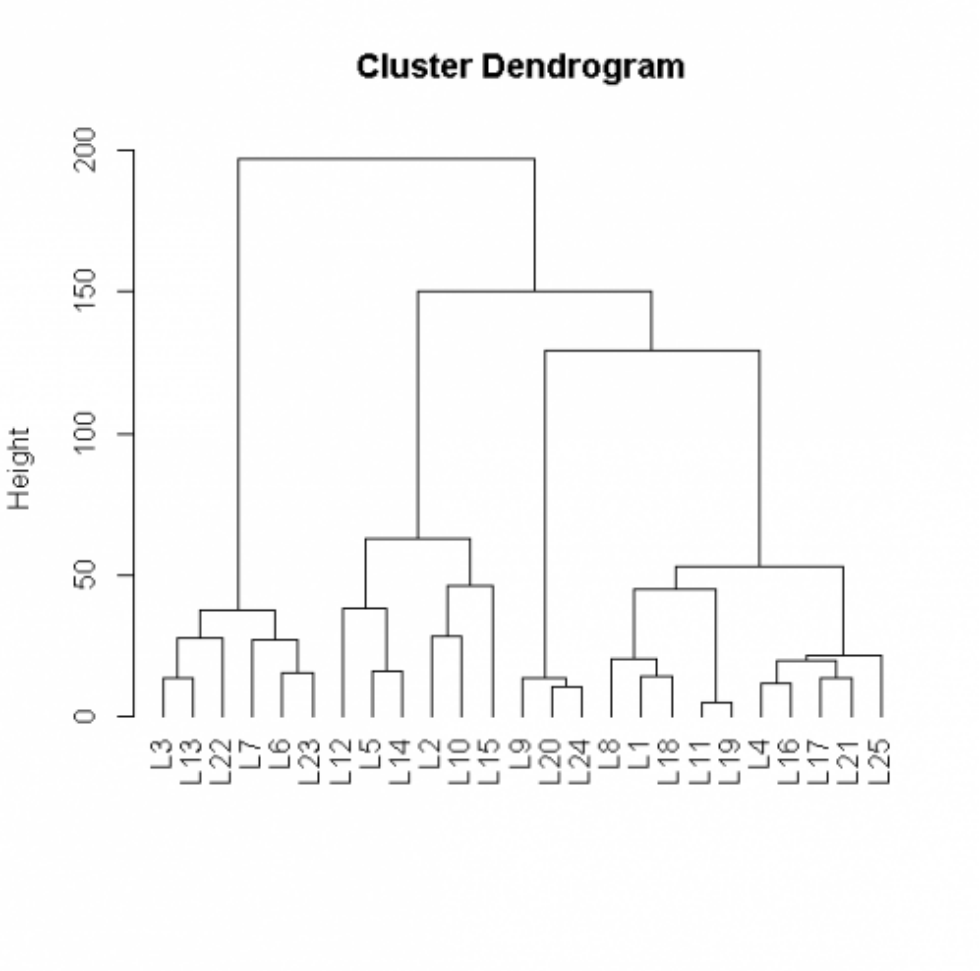
```
> save(nVar,nVarP,so,numSO,SOs,file="./sr25/sr25.so")
> date()
[1] "Sat Nov 03 07:11:15 2012"
> alpha <-rep(1/nVar,nVar)
> rez <- leaderSO(SOs,25)
Step 1
clust
   1    2    3    4    5    6    7    8    9   10   11   12   13   14   15   16
 130 1075  602   96  375  882  379   28  501  237  168  857  334  175  272  179
  17   18   19   20   21   22   23   24   25
 581  137   78   88  277  143  165  269  166
 [1] 0.4424408 0.4596538 0.4499387 0.4489372 0.4470013 0.4753601 0.4577974
 [8] 0.4397338 0.4697205 0.4506480 0.4472091 0.4817797 0.4512397 0.4443368
[15] 0.4435127 0.4418945 0.4802104 0.4537058 0.4458928 0.4456002 0.4613981
[22] 0.4412230 0.4523715 0.4399890 0.4569876
 [1] -0.4424408 -0.4596538 -0.4499387 -0.4489372 -0.4470013 -0.4753601
 [7] -0.4577974 -0.4397338 -0.4697205 -0.4506480 -0.4472091 -0.4817797
[13] -0.4512397 -0.4443368 -0.4435127 -0.4418945 -0.4802104 -0.4537058
[19] -0.4458928 -0.4456002 -0.4613981 -0.4412230 -0.4523715 -0.4399890
[25] -0.4569876
 [1]  54.07908 450.00058 252.98951  39.45177 155.26080 362.11904 156.06820
 [8]  11.64665 209.99214  99.61139  69.49693 359.51359 139.47882  73.29974
[15] 113.63847  73.40548 242.24122  57.69107  32.77622  36.53021 116.37494
[22]  59.30112  68.02095 110.01321  69.56174
[1] 3412.563
Times repeat = 10

Step 2
clust
  1   2   3   4   5   6   7   8   9  10  11  12  13  14  15  16  17  18  19  20
234 992 510 161 222 762 309  86 601 232 237 837 173 364 224 153 198 201 140  90
 21  22  23  24  25
461 320 259 115 313
```

```
.........................................

[22] 136.36349  93.83314  69.10369  96.68143
[1] 2477.077

Step 69
clust
  1   2   3   4   5   6   7   8   9  10  11  12  13  14  15  16  17  18  19  20
330 600 266 286 203 500 430 381 357 459 179 771 324 356 136 216 149 331 101 147
 21  22  23  24  25
268 462 329 286 327
 [1] 0.4404389 0.4563706 0.4399778 0.4475609 0.4636173 0.4234320 0.4580795
 [8] 0.4547127 0.3978984 0.4588445 0.3687990 0.4686583 0.4622807 0.4559260
[15] 0.4426157 0.4374157 0.4350053 0.4663559 0.3511556 0.4381077 0.4347615
[22] 0.4146484 0.4320133 0.4280194 0.4651733
 [1] 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 [1] 109.17241 157.86730  89.48315  98.65276  59.81671 141.87021 126.43962
 [8] 134.96135  71.08819 145.83863  36.53670 265.04374 120.18657 122.27654
[15]  20.18357  62.41475  47.59801 126.56725  20.70570  43.90852  80.48392
[22] 136.36349  93.83314  69.10369  96.68143
[1] 2477.077
Times repeat = 0
> save(rez,file="./sr25/sr25.rez")
> hc <- hclustSO(rez$leaders)
> plot(hc,hang=-1)
> long[rez$clust==19]
  [1] "ARCHWAY HOME STYLE COOKIES,SUGAR FREE OATMEAL"
  [2] "ARCHWAY Home Style Cookies, Chocolate Chip Ice Box"
  [3] "ARCHWAY Home Style Cookies, Date Filled Oatmeal"
  [4] "ARCHWAY Home Style Cookies, Dutch Cocoa"
  [5] "ARCHWAY HOME STYLE COOKIES,FROSTY LEMON"
  [6] "ARCHWAY Home Style Cookies, Iced Molasses"
  [7] "ARCHWAY Home Style Cookies, Iced Oatmeal"
  [8] "ARCHWAY Home Style Cookies, Molasses"
.......
 [93] "AUSTIN,CHEDDAR CHS ON WAFER CRACKERS,SANDWICH-TYPE"
 [94] "KEEBLER,CHS & PNUT BUTTER SNDWCH CRACKERS"
 [95] "KEEBLER,SUGAR CONES"
 [96] "MURRAY,HONEY GRAHAM"
 [97] "SUNSHINE,CHEEZ-IT,ORIGINAL CRACKERS"
 [98] "SUNSHINE,CHEEZ-IT,RED FAT CRACKERS"
 [99] "SUNSHINE,KRISPY,SOUP & OYSTER CRACKERS (LARGE)"
[100] "KEEBLER,ZESTA,SALTINES,ORIGINAL"
[101] "KEEBLER,ZESTA,SALTINES W/ WHL WHEAT"
>
```



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