Dimensionality reduction

Exercices

PCA

```
library(mixOmics)
```

1. Load the `nutrimouse` data from the `mixOmics` R package and investigate its structure. A data object provided by an R package can be loaded with `data`. Its structure can be obainted with `str`, `length`, `dim`, etc.

```
data("nutrimouse")
## display the structure of the nutrimouse object
str(nutrimouse)
```

```
## List of 4
##  $ gene    :'data.frame':    40 obs. of  120 variables:
##   ..$ X36b4    : num [1:40] -0.42 -0.44 -0.48 -0.45 -0.42 -0.43 -0.53 -0.49 -0.36 -0.5 ...
##   ..$ ACAT1    : num [1:40] -0.65 -0.68 -0.74 -0.69 -0.71 -0.69 -0.62 -0.69 -0.66 -0.62 ...
##   ..$ ACAT2    : num [1:40] -0.84 -0.91 -1.1 -0.65 -0.54 -0.8 -1 -0.91 -0.74 -0.79 ...
##   ..$ ACBP     : num [1:40] -0.34 -0.32 -0.46 -0.41 -0.38 -0.32 -0.44 -0.37 -0.39 -0.36 ...
##   ..$ ACC1     : num [1:40] -1.29 -1.23 -1.3 -1.26 -1.21 -1.13 -1.22 -1.29 -1.15 -1.21 ...
##   ..$ ACC2     : num [1:40] -1.13 -1.06 -1.09 -1.09 -0.89 -0.79 -1 -1.06 -1.08 -0.82 ...
##   ..$ ACOTH    : num [1:40] -0.93 -0.99 -1.06 -0.93 -1 -0.93 -0.94 -1.05 -0.88 -0.92 ...
##   ..$ ADISP    : num [1:40] -0.98 -0.97 -1.08 -1.02 -0.95 -0.97 -0.94 -1.02 -0.98 -0.99 ...
##   ..$ ADSS1    : num [1:40] -1.19 -1 -1.18 -1.07 -1.08 -1.07 -1.05 -1.16 -1.05 -1 ...
##   ..$ ALDH3    : num [1:40] -0.68 -0.62 -0.75 -0.71 -0.76 -0.75 -0.67 -0.75 -0.66 -0.69 ...
##   ..$ AM2R     : num [1:40] -0.59 -0.58 -0.66 -0.65 -0.59 -0.55 -0.66 -0.66 -0.53 -0.62 ...
##   ..$ AOX      : num [1:40] -0.16 -0.12 -0.16 -0.17 -0.31 -0.23 -0.09 -0.22 -0.06 -0.23 ...
##   ..$ BACT     : num [1:40] -0.22 -0.32 -0.32 -0.32 -0.31 -0.29 -0.25 -0.21 -0.15 -0.2 ...
##   ..$ BIEN     : num [1:40] -0.89 -0.88 -0.89 -0.77 -0.97 -0.84 -0.86 -0.9 -0.74 -0.76 ...
##   ..$ BSEP     : num [1:40] -0.69 -0.6 -0.7 -0.67 -0.68 -0.55 -0.67 -0.66 -0.6 -0.58 ...
##   ..$ Bcl.3    : num [1:40] -1.18 -1.07 -1.17 -1.12 -0.93 -1.08 -1.03 -1.01 -1.01 -1.1 ...
##   ..$ C16SR    : num [1:40] 1.66 1.65 1.57 1.61 1.66 1.7 1.58 1.62 1.72 1.55 ...
##   ..$ CACP     : num [1:40] -0.92 -0.87 -1.02 -0.89 -0.93 -0.97 -0.97 -0.96 -0.85 -0.95 ...
##   ..$ CAR1     : num [1:40] -0.97 -0.92 -0.98 -0.97 -1.06 -1.03 -0.91 -1.11 -0.85 -0.99 ...
##   ..$ CBS      : num [1:40] -0.26 -0.36 -0.4 -0.39 -0.35 -0.31 -0.32 -0.4 -0.26 -0.39 ...
##   ..$ CIDEA    : num [1:40] -1.21 -1.17 -1.29 -1.18 -1.15 -1.14 -1.16 -1.26 -1.12 -1.08 ...
##   ..$ COX1     : num [1:40] -1.11 -1.06 -1.17 -1.03 -0.99 -1.03 -1.15 -1.18 -0.94 -1.07 ...
##   ..$ COX2     : num [1:40] -1.18 -1.06 -1.14 -1.13 -1.1 -1.16 -1.06 -1.24 -1.23 -1.09 ...
##   ..$ CPT2     : num [1:40] -0.87 -0.87 -0.95 -0.88 -0.91 -0.92 -0.86 -0.93 -0.82 -0.88 ...
##   ..$ CYP24    : num [1:40] -1.37 -1.14 -1.3 -1.27 -1.2 -1.11 -1.12 -1.3 -1.14 -1.08 ...
##   ..$ CYP26    : num [1:40] -1.21 -1.12 -1.22 -1.18 -1.16 -1.1 -1.07 -1.23 -1.1 -1.1 ...
##   ..$ CYP27a1  : num [1:40] -0.71 -0.62 -0.78 -0.71 -0.69 -0.6 -0.69 -0.81 -0.62 -0.62 ...
##   ..$ CYP27b1  : num [1:40] -1.31 -1.14 -1.29 -1.27 -1.2 -1.15 -1.17 -1.28 -1.13 -1.15 ...
##   ..$ CYP2b10  : num [1:40] -1.23 -1.2 -1.32 -1.23 -1.22 -1.1 -1.07 -1.26 -1.19 -1.1 ...
```

```
##   ..$ CYP2b13  : num [1:40] -1.19 -1.06 -1.25 -1.13 -1.1 -1.07 -1.2 -1.37 -1.15 -1.11 ...
##   ..$ CYP2c29  : num [1:40] -0.06 -0.2 -0.3 -0.07 -0.29 -0.28 -0.1 -0.1 0.18 -0.33 ...
##   ..$ CYP3A11  : num [1:40] -0.09 -0.34 -0.45 -0.11 -0.51 -0.55 -0.18 -0.25 0.06 -0.4 ...
##   ..$ CYP4A10  : num [1:40] -0.81 -0.88 -0.71 -0.65 -1.16 -0.99 -0.62 -0.82 -0.48 -0.79 ...
##   ..$ CYP4A14  : num [1:40] -0.81 -0.84 -0.98 -0.41 -1.16 -1.09 -0.76 -0.87 -0.37 -0.95 ...
##   ..$ CYP7a    : num [1:40] -0.77 -0.71 -0.93 -0.8 -0.71 -0.74 -0.76 -0.88 -0.77 -0.77 ...
##   ..$ CYP8b1   : num [1:40] -0.77 -0.63 -0.53 -0.73 -0.51 -0.55 -0.57 -0.63 -0.6 -0.66 ...
##   ..$ FAS      : num [1:40] -0.41 -0.37 -0.3 -0.59 -0.06 0.18 -0.16 0.04 -0.53 0.08 ...
##   ..$ FAT      : num [1:40] -1.03 -0.98 -1.03 -1.06 -0.99 -0.99 -0.89 -1.08 -1.04 -0.91 ...
##   ..$ FDFT     : num [1:40] -0.98 -0.92 -1.04 -1 -0.99 -1 -1.02 -0.97 -1.03 -0.95 ...
##   ..$ FXR      : num [1:40] -0.93 -0.87 -1 -0.9 -0.89 -0.89 -0.86 -1.01 -0.81 -0.91 ...
##   ..$ G6PDH    : num [1:40] -1.22 -1.09 -1.28 -1.19 -1.16 -0.96 -1.15 -1.26 -1.13 -1.03 ...
##   ..$ G6Pase   : num [1:40] -0.46 -0.63 -1.06 -0.71 -0.58 -0.49 -0.51 -0.61 -0.38 -0.6 ...
##   ..$ GK       : num [1:40] -0.71 -0.67 -0.68 -0.75 -0.62 -0.59 -0.59 -0.66 -0.68 -0.47 ...
##   ..$ GS       : num [1:40] -1.24 -1.22 -1.36 -1.21 -1.22 -1.16 -1.15 -1.31 -1.16 -1.19 ...
##   ..$ GSTa     : num [1:40] 0 -0.05 -0.13 -0.09 -0.02 -0.11 -0.06 -0.04 0.03 -0.02 ...
##   ..$ GSTmu    : num [1:40] 0.02 -0.05 -0.19 0.03 -0.23 -0.05 -0.22 -0.07 0.23 -0.14 ...
##   ..$ GSTpi2   : num [1:40] 0.45 0.3 0.18 0.36 0.3 0.17 0.12 0.48 0.53 0.01 ...
##   ..$ HMGCoAred: num [1:40] -0.95 -0.86 -0.96 -1.02 -0.7 -0.76 -1 -0.88 -0.96 -0.7 ...
##   ..$ HPNCL    : num [1:40] -0.65 -0.69 -0.75 -0.61 -0.66 -0.56 -0.61 -0.71 -0.53 -0.6 ...
##   ..$ IL.2     : num [1:40] -0.94 -0.94 -1.16 -0.97 -0.93 -0.96 -0.96 -0.85 -0.84 -0.95 ...
##   ..$ L.FABP   : num [1:40] 0.24 0.27 0.17 0.16 0 0.23 0.18 0.18 0.2 0.2 ...
##   ..$ LCE      : num [1:40] 0.09 0.06 -0.05 0.01 -0.07 -0.1 -0.03 -0.08 0.12 -0.1 ...
##   ..$ LDLr     : num [1:40] -0.82 -0.68 -0.82 -0.94 -0.73 -0.74 -0.8 -0.83 -0.81 -0.72 ...
##   ..$ LPK      : num [1:40] -0.32 -0.39 -0.38 -0.38 -0.17 -0.14 -0.35 -0.13 -0.32 -0.24 ...
##   ..$ LPL      : num [1:40] -1.01 -0.97 -1.11 -0.99 -1.05 -0.99 -0.93 -1.07 -0.94 -0.95 ...
##   ..$ LXRa     : num [1:40] -0.82 -0.82 -0.91 -0.85 -0.83 -0.79 -0.77 -0.84 -0.75 -0.78 ...
##   ..$ LXRb     : num [1:40] -1 -0.95 -1.16 -1.01 -1.01 -0.99 -0.98 -1.04 -0.98 -0.99 ...
##   ..$ Lpin     : num [1:40] -0.87 -0.97 -0.95 -1 -0.57 -0.51 -0.81 -0.83 -0.83 -0.48 ...
##   ..$ Lpin1    : num [1:40] -0.85 -0.99 -0.94 -1.02 -0.53 -0.51 -0.81 -0.87 -0.82 -0.49 ...
##   ..$ Lpin2    : num [1:40] -0.85 -0.87 -0.9 -0.88 -0.72 -0.68 -0.8 -0.9 -0.68 -0.67 ...
##   ..$ Lpin3    : num [1:40] -1.23 -1.12 -1.25 -1.18 -1.12 -1.09 -1.04 -1.23 -1.13 -1.11 ...
##   ..$ M.CPT1   : num [1:40] -1.15 -1.06 -1.26 -1.1 -1.11 -1.14 -1.08 -1.19 -1.06 -1.09 ...
##   ..$ MCAD     : num [1:40] -0.6 -0.62 -0.7 -0.59 -0.69 -0.66 -0.53 -0.66 -0.45 -0.62 ...
##   ..$ MDR1     : num [1:40] -1.15 -1.1 -1.26 -1.13 -1.11 -1.09 -1.09 -1.19 -1.06 -1.1 ...
##   ..$ MDR2     : num [1:40] -0.77 -0.65 -0.86 -0.77 -0.7 -0.69 -0.81 -0.81 -0.69 -0.75 ...
##   ..$ MRP6     : num [1:40] -0.99 -0.85 -0.9 -0.95 -0.91 -0.84 -0.88 -1.02 -0.83 -0.86 ...
##   ..$ MS       : num [1:40] -1.11 -1.06 -1.2 -1.09 -1.09 -1.09 -0.99 -1.16 -1.06 -0.98 ...
##   ..$ MTHFR    : num [1:40] -0.96 -0.99 -1.1 -0.95 -0.93 -0.96 -0.88 -1.03 -1.01 -0.95 ...
##   ..$ NGFiB    : num [1:40] -1.21 -1.08 -1.24 -1.12 -1.11 -1.04 -1.02 -1.21 -1.11 -1.04 ...
##   ..$ NURR1    : num [1:40] -1.21 -1.1 -1.32 -1.11 -1.14 -1.18 -1.1 -1.26 -1.14 -1.09 ...
##   ..$ Ntcp     : num [1:40] -0.49 -0.45 -0.44 -0.54 -0.47 -0.46 -0.55 -0.5 -0.44 -0.43 ...
##   ..$ OCTN2    : num [1:40] -1.15 -1.15 -1.2 -1.17 -1.19 -1.11 -1.08 -1.21 -1.05 -1.08 ...
##   ..$ PAL      : num [1:40] -1.32 -1.25 -1.16 -1.25 -1.24 -1.02 -1.04 -1.27 -0.93 -0.92 ...
##   ..$ PDK4     : num [1:40] -1.16 -1.16 -1.27 -1.16 -1.13 -1.08 -1.14 -1.24 -1.19 -1.04 ...
##   ..$ PECI     : num [1:40] -0.68 -0.69 -0.92 -0.71 -0.83 -0.81 -0.79 -0.85 -0.58 -0.82 ...
##   ..$ PLTP     : num [1:40] -1.1 -0.99 -1.03 -1.08 -0.98 -0.89 -1.05 -1.07 -1.02 -0.85 ...
##   ..$ PMDCI    : num [1:40] -0.52 -0.52 -0.6 -0.52 -0.71 -0.69 -0.55 -0.57 -0.46 -0.69 ...
##   ..$ PON      : num [1:40] -0.52 -0.55 -0.65 -0.64 -0.57 -0.63 -0.56 -0.65 -0.6 -0.64 ...
##   ..$ PPARa    : num [1:40] -0.93 -0.86 -0.95 -0.97 -0.94 -0.95 -0.9 -1.12 -0.88 -0.95 ...
##   ..$ PPARd    : num [1:40] -1.51 -1.59 -1.71 -1.57 -1.53 -1.56 -1.49 -1.57 -1.58 -1.54 ...
##   ..$ PPARg    : num [1:40] -1.06 -1.02 -1.14 -1.05 -1.09 -1.01 -1 -1.13 -0.97 -1.07 ...
##   ..$ PXR      : num [1:40] -0.99 -0.96 -1.1 -0.99 -1 -1.03 -0.93 -1.07 -0.98 -0.96 ...
##   ..$ Pex11a   : num [1:40] -1 -1.02 -1.2 -1 -0.95 -1.07 -1.05 -1.02 -1 -1.01 ...
```

```
##   ..$ RARa     : num [1:40] -1.2 -1.06 -1.16 -1.17 -1.15 -1.13 -1.09 -1.24 -1.03 -1.09 ...
##   ..$ RARb2    : num [1:40] -1.19 -1.11 -1.23 -1.16 -1.14 -1.07 -1.09 -1.18 -1.12 -1.1 ...
##   ..$ RXRa     : num [1:40] -0.67 -0.59 -0.68 -0.72 -0.78 -0.62 -0.65 -0.76 -0.55 -0.67 ...
##   ..$ RXRb2    : num [1:40] -0.95 -0.95 -1.07 -0.95 -0.98 -0.94 -0.92 -1.03 -0.94 -0.95 ...
##   ..$ RXRg1    : num [1:40] -1.16 -1.1 -1.21 -1.1 -1.11 -1.03 -1.07 -1.19 -1.05 -1.04 ...
##   ..$ S14      : num [1:40] -0.93 -0.86 -0.84 -1.05 -0.65 -0.4 -0.73 -0.62 -0.99 -0.25 ...
##   ..$ SHP1     : num [1:40] -1.1 -0.97 -1.09 -1.03 -1.13 -0.98 -0.95 -1.21 -0.93 -0.97 ...
##   ..$ SIAT4c   : num [1:40] -1.07 -0.97 -1.04 -0.99 -0.94 -0.93 -0.89 -1.04 -0.93 -0.95 ...
##   ..$ SPI1.1   : num [1:40] 1.19 1.15 1.09 1.07 1.22 1.05 1.15 1.18 1.21 1.04 ...
##   ..$ SR.BI    : num [1:40] -0.84 -0.86 -0.95 -0.95 -1.06 -0.8 -0.83 -1 -0.83 -0.77 ...
##   ..$ THB      : num [1:40] -0.79 -0.85 -0.92 -0.79 -0.84 -0.86 -0.8 -0.86 -0.83 -0.85 ...
##   ..$ THIOL    : num [1:40] -0.18 -0.15 -0.24 -0.15 -0.35 -0.29 -0.22 -0.23 -0.17 -0.18 ...
##   ..$ TRa      : num [1:40] -1.48 -1.46 -1.58 -1.54 -1.46 -1.44 -1.32 -1.56 -1.46 -1.35 ...
##   ..$ TRb      : num [1:40] -1.07 -1 -1.16 -1.11 -1.01 -1 -0.97 -1.08 -1.02 -0.98 ...
##   ..$ Tpalpha  : num [1:40] -0.69 -0.74 -0.81 -0.74 -0.82 -0.76 -0.72 -0.76 -0.65 -0.83 ...
##   ..$ Tpbeta   : num [1:40] -1.11 -1.09 -1.14 -1.04 -1.2 -1.05 -1 -1.16 -0.91 -1.07 ...
##   .. [list output truncated]
##  $ lipid   :'data.frame':    40 obs. of  21 variables:
##   ..$ C14.0   : num [1:40] 0.34 0.38 0.36 0.22 0.37 1.7 0.35 0.34 0.22 1.38 ...
##   ..$ C16.0   : num [1:40] 26.4 24 23.7 25.5 24.8 ...
##   ..$ C18.0   : num [1:40] 10.22 9.93 8.96 8.14 9.63 ...
##   ..$ C16.1n.9: num [1:40] 0.35 0.55 0.55 0.49 0.46 0.66 0.36 0.29 0.44 0.9 ...
##   ..$ C16.1n.7: num [1:40] 3.1 2.54 2.65 2.82 2.85 7.26 3.6 3.27 2.36 7.01 ...
##   ..$ C18.1n.9: num [1:40] 17 20.1 22.9 21.9 21.4 ...
##   ..$ C18.1n.7: num [1:40] 2.41 3.92 3.96 2.52 2.96 8.99 2.15 1.99 1.81 8.85 ...
##   ..$ C20.1n.9: num [1:40] 0.26 0.23 0.26 0 0.3 0.36 0.25 0.31 0 0.21 ...
##   ..$ C20.3n.9: num [1:40] 0 0 0.19 0 0.27 2.89 0 0 0 2.03 ...
##   ..$ C18.2n.6: num [1:40] 8.93 14.98 16.06 13.89 14.55 ...
##   ..$ C18.3n.6: num [1:40] 0 0.3 0.27 0 0.27 2.66 0 0 0 0 ...
##   ..$ C20.2n.6: num [1:40] 0 0.3 0.33 0 0.23 0 0 0 0 0 ...
##   ..$ C20.3n.6: num [1:40] 0.78 1.64 1.51 1.1 1.58 0.81 0.68 0.72 1.07 0.59 ...
##   ..$ C20.4n.6: num [1:40] 3.07 15.34 13.27 3.92 11.85 ...
##   ..$ C22.4n.6: num [1:40] 0 0.58 0.54 0 0.32 0 0 0 0 0 ...
##   ..$ C22.5n.6: num [1:40] 0 2.1 1.77 0 0.44 0.56 0 0 0 0.39 ...
##   ..$ C18.3n.3: num [1:40] 5.97 0 0 0.49 0.42 0 8.4 6.01 0.55 0 ...
##   ..$ C20.3n.3: num [1:40] 0.37 0 0 0 0 0 0.42 0.39 0 0 ...
##   ..$ C20.5n.3: num [1:40] 8.62 0 0 2.99 0.3 0 7.37 7.96 3.13 0 ...
##   ..$ C22.5n.3: num [1:40] 1.75 0.48 0.22 1.04 0.35 2.13 2.05 2.33 1.65 0 ...
##   ..$ C22.6n.3: num [1:40] 10.39 2.61 2.51 14.99 6.69 ...
##  $ diet    : Factor w/ 5 levels "coc","fish","lin",..: 3 5 5 2 4 1 3 3 2 1 ...
##  $ genotype: Factor w/ 2 levels "wt","ppar": 1 1 1 1 1 1 1 1 1 1 ...
```

```
## check dimensions
lapply(nutrimouse, dim) # apply function dim to each element in list nutrimouse
```

```
## $gene
## [1]  40 120
##
## $lipid
## [1] 40 21
##
## $diet
## NULL
##
## $genotype
```

```
## NULL
```

```
lapply(nutrimouse, length) # apply function length to each element in list nutrimouse
```

```
## $gene
## [1] 120
##
## $lipid
## [1] 21
##
## $diet
## [1] 40
##
## $genotype
## [1] 40
```

```
## get gene expression data structure
str(nutrimouse$gene)
```

2. Take the gene expression dataset in *samples* x *variables* matrix format. Investigate their distribution.

```
## 'data.frame':    40 obs. of  120 variables:
##  $ X36b4    : num  -0.42 -0.44 -0.48 -0.45 -0.42 -0.43 -0.53 -0.49 -0.36 -0.5 ...
##  $ ACAT1    : num  -0.65 -0.68 -0.74 -0.69 -0.71 -0.69 -0.62 -0.69 -0.66 -0.62 ...
##  $ ACAT2    : num  -0.84 -0.91 -1.1 -0.65 -0.54 -0.8 -1 -0.91 -0.74 -0.79 ...
##  $ ACBP     : num  -0.34 -0.32 -0.46 -0.41 -0.38 -0.32 -0.44 -0.37 -0.39 -0.36 ...
##  $ ACC1     : num  -1.29 -1.23 -1.3 -1.26 -1.21 -1.13 -1.22 -1.29 -1.15 -1.21 ...
##  $ ACC2     : num  -1.13 -1.06 -1.09 -1.09 -0.89 -0.79 -1 -1.06 -1.08 -0.82 ...
##  $ ACOTH    : num  -0.93 -0.99 -1.06 -0.93 -1 -0.93 -0.94 -1.05 -0.88 -0.92 ...
##  $ ADISP    : num  -0.98 -0.97 -1.08 -1.02 -0.95 -0.97 -0.94 -1.02 -0.98 -0.99 ...
##  $ ADSS1    : num  -1.19 -1 -1.18 -1.07 -1.08 -1.07 -1.05 -1.16 -1.05 -1 ...
##  $ ALDH3    : num  -0.68 -0.62 -0.75 -0.71 -0.76 -0.75 -0.67 -0.75 -0.66 -0.69 ...
##  $ AM2R     : num  -0.59 -0.58 -0.66 -0.65 -0.59 -0.55 -0.66 -0.66 -0.53 -0.62 ...
##  $ AOX      : num  -0.16 -0.12 -0.16 -0.17 -0.31 -0.23 -0.09 -0.22 -0.06 -0.23 ...
##  $ BACT     : num  -0.22 -0.32 -0.32 -0.32 -0.31 -0.29 -0.25 -0.21 -0.15 -0.2 ...
##  $ BIEN     : num  -0.89 -0.88 -0.89 -0.77 -0.97 -0.84 -0.86 -0.9 -0.74 -0.76 ...
##  $ BSEP     : num  -0.69 -0.6 -0.7 -0.67 -0.68 -0.55 -0.67 -0.66 -0.6 -0.58 ...
##  $ Bcl.3    : num  -1.18 -1.07 -1.17 -1.12 -0.93 -1.08 -1.03 -1.01 -1.01 -1.1 ...
##  $ C16SR    : num  1.66 1.65 1.57 1.61 1.66 1.7 1.58 1.62 1.72 1.55 ...
##  $ CACP     : num  -0.92 -0.87 -1.02 -0.89 -0.93 -0.97 -0.97 -0.96 -0.85 -0.95 ...
##  $ CAR1     : num  -0.97 -0.92 -0.98 -0.97 -1.06 -1.03 -0.91 -1.11 -0.85 -0.99 ...
##  $ CBS      : num  -0.26 -0.36 -0.4 -0.39 -0.35 -0.31 -0.32 -0.4 -0.26 -0.39 ...
##  $ CIDEA    : num  -1.21 -1.17 -1.29 -1.18 -1.15 -1.14 -1.16 -1.26 -1.12 -1.08 ...
##  $ COX1     : num  -1.11 -1.06 -1.17 -1.03 -0.99 -1.03 -1.15 -1.18 -0.94 -1.07 ...
##  $ COX2     : num  -1.18 -1.06 -1.14 -1.13 -1.1 -1.16 -1.06 -1.24 -1.23 -1.09 ...
##  $ CPT2     : num  -0.87 -0.87 -0.95 -0.88 -0.91 -0.92 -0.86 -0.93 -0.82 -0.88 ...
##  $ CYP24    : num  -1.37 -1.14 -1.3 -1.27 -1.2 -1.11 -1.12 -1.3 -1.14 -1.08 ...
##  $ CYP26    : num  -1.21 -1.12 -1.22 -1.18 -1.16 -1.1 -1.07 -1.23 -1.1 -1.1 ...
##  $ CYP27a1  : num  -0.71 -0.62 -0.78 -0.71 -0.69 -0.6 -0.69 -0.81 -0.62 -0.62 ...
##  $ CYP27b1  : num  -1.31 -1.14 -1.29 -1.27 -1.2 -1.15 -1.17 -1.28 -1.13 -1.15 ...
##  $ CYP2b10  : num  -1.23 -1.2 -1.32 -1.23 -1.22 -1.1 -1.07 -1.26 -1.19 -1.1 ...
##  $ CYP2b13  : num  -1.19 -1.06 -1.25 -1.13 -1.1 -1.07 -1.2 -1.37 -1.15 -1.11 ...
##  $ CYP2c29  : num  -0.06 -0.2 -0.3 -0.07 -0.29 -0.28 -0.1 -0.1 0.18 -0.33 ...
```

```
##  $ CYP3A11  : num  -0.09 -0.34 -0.45 -0.11 -0.51 -0.55 -0.18 -0.25 0.06 -0.4 ...
##  $ CYP4A10  : num  -0.81 -0.88 -0.71 -0.65 -1.16 -0.99 -0.62 -0.82 -0.48 -0.79 ...
##  $ CYP4A14  : num  -0.81 -0.84 -0.98 -0.41 -1.16 -1.09 -0.76 -0.87 -0.37 -0.95 ...
##  $ CYP7a    : num  -0.77 -0.71 -0.93 -0.8 -0.71 -0.74 -0.76 -0.88 -0.77 -0.77 ...
##  $ CYP8b1   : num  -0.77 -0.63 -0.53 -0.73 -0.51 -0.55 -0.57 -0.63 -0.6 -0.66 ...
##  $ FAS      : num  -0.41 -0.37 -0.3 -0.59 -0.06 0.18 -0.16 0.04 -0.53 0.08 ...
##  $ FAT      : num  -1.03 -0.98 -1.03 -1.06 -0.99 -0.99 -0.89 -1.08 -1.04 -0.91 ...
##  $ FDFT     : num  -0.98 -0.92 -1.04 -1 -0.99 -1 -1.02 -0.97 -1.03 -0.95 ...
##  $ FXR      : num  -0.93 -0.87 -1 -0.9 -0.89 -0.89 -0.86 -1.01 -0.81 -0.91 ...
##  $ G6PDH    : num  -1.22 -1.09 -1.28 -1.19 -1.16 -0.96 -1.15 -1.26 -1.13 -1.03 ...
##  $ G6Pase   : num  -0.46 -0.63 -1.06 -0.71 -0.58 -0.49 -0.51 -0.61 -0.38 -0.6 ...
##  $ GK       : num  -0.71 -0.67 -0.68 -0.75 -0.62 -0.59 -0.59 -0.66 -0.68 -0.47 ...
##  $ GS       : num  -1.24 -1.22 -1.36 -1.21 -1.22 -1.16 -1.15 -1.31 -1.16 -1.19 ...
##  $ GSTa     : num  0 -0.05 -0.13 -0.09 -0.02 -0.11 -0.06 -0.04 0.03 -0.02 ...
##  $ GSTmu    : num  0.02 -0.05 -0.19 0.03 -0.23 -0.05 -0.22 -0.07 0.23 -0.14 ...
##  $ GSTpi2   : num  0.45 0.3 0.18 0.36 0.3 0.17 0.12 0.48 0.53 0.01 ...
##  $ HMGCoAred: num  -0.95 -0.86 -0.96 -1.02 -0.7 -0.76 -1 -0.88 -0.96 -0.7 ...
##  $ HPNCL    : num  -0.65 -0.69 -0.75 -0.61 -0.66 -0.56 -0.61 -0.71 -0.53 -0.6 ...
##  $ IL.2     : num  -0.94 -0.94 -1.16 -0.97 -0.93 -0.96 -0.96 -0.85 -0.84 -0.95 ...
##  $ L.FABP   : num  0.24 0.27 0.17 0.16 0 0.23 0.18 0.18 0.2 0.2 ...
##  $ LCE      : num  0.09 0.06 -0.05 0.01 -0.07 -0.1 -0.03 -0.08 0.12 -0.1 ...
##  $ LDLr     : num  -0.82 -0.68 -0.82 -0.94 -0.73 -0.74 -0.8 -0.83 -0.81 -0.72 ...
##  $ LPK      : num  -0.32 -0.39 -0.38 -0.38 -0.17 -0.14 -0.35 -0.13 -0.32 -0.24 ...
##  $ LPL      : num  -1.01 -0.97 -1.11 -0.99 -1.05 -0.99 -0.93 -1.07 -0.94 -0.95 ...
##  $ LXRa     : num  -0.82 -0.82 -0.91 -0.85 -0.83 -0.79 -0.77 -0.84 -0.75 -0.78 ...
##  $ LXRb     : num  -1 -0.95 -1.16 -1.01 -1.01 -0.99 -0.98 -1.04 -0.98 -0.99 ...
##  $ Lpin     : num  -0.87 -0.97 -0.95 -1 -0.57 -0.51 -0.81 -0.83 -0.83 -0.48 ...
##  $ Lpin1    : num  -0.85 -0.99 -0.94 -1.02 -0.53 -0.51 -0.81 -0.87 -0.82 -0.49 ...
##  $ Lpin2    : num  -0.85 -0.87 -0.9 -0.88 -0.72 -0.68 -0.8 -0.9 -0.68 -0.67 ...
##  $ Lpin3    : num  -1.23 -1.12 -1.25 -1.18 -1.12 -1.09 -1.04 -1.23 -1.13 -1.11 ...
##  $ M.CPT1   : num  -1.15 -1.06 -1.26 -1.1 -1.11 -1.14 -1.08 -1.19 -1.06 -1.09 ...
##  $ MCAD     : num  -0.6 -0.62 -0.7 -0.59 -0.69 -0.66 -0.53 -0.66 -0.45 -0.62 ...
##  $ MDR1     : num  -1.15 -1.1 -1.26 -1.13 -1.11 -1.09 -1.09 -1.19 -1.06 -1.1 ...
##  $ MDR2     : num  -0.77 -0.65 -0.86 -0.77 -0.7 -0.69 -0.81 -0.81 -0.69 -0.75 ...
##  $ MRP6     : num  -0.99 -0.85 -0.9 -0.95 -0.91 -0.84 -0.88 -1.02 -0.83 -0.86 ...
##  $ MS       : num  -1.11 -1.06 -1.2 -1.09 -1.09 -1.09 -0.99 -1.16 -1.06 -0.98 ...
##  $ MTHFR    : num  -0.96 -0.99 -1.1 -0.95 -0.93 -0.96 -0.88 -1.03 -1.01 -0.95 ...
##  $ NGFiB    : num  -1.21 -1.08 -1.24 -1.12 -1.11 -1.04 -1.02 -1.21 -1.11 -1.04 ...
##  $ NURR1    : num  -1.21 -1.1 -1.32 -1.11 -1.14 -1.18 -1.1 -1.26 -1.14 -1.09 ...
##  $ Ntcp     : num  -0.49 -0.45 -0.44 -0.54 -0.47 -0.46 -0.55 -0.5 -0.44 -0.43 ...
##  $ OCTN2    : num  -1.15 -1.15 -1.2 -1.17 -1.19 -1.11 -1.08 -1.21 -1.05 -1.08 ...
##  $ PAL      : num  -1.32 -1.25 -1.16 -1.25 -1.24 -1.02 -1.04 -1.27 -0.93 -0.92 ...
##  $ PDK4     : num  -1.16 -1.16 -1.27 -1.16 -1.13 -1.08 -1.14 -1.24 -1.19 -1.04 ...
##  $ PECI     : num  -0.68 -0.69 -0.92 -0.71 -0.83 -0.81 -0.79 -0.85 -0.58 -0.82 ...
##  $ PLTP     : num  -1.1 -0.99 -1.03 -1.08 -0.98 -0.89 -1.05 -1.07 -1.02 -0.85 ...
##  $ PMDCI    : num  -0.52 -0.52 -0.6 -0.52 -0.71 -0.69 -0.55 -0.57 -0.46 -0.69 ...
##  $ PON      : num  -0.52 -0.55 -0.65 -0.64 -0.57 -0.63 -0.56 -0.65 -0.6 -0.64 ...
##  $ PPARa    : num  -0.93 -0.86 -0.95 -0.97 -0.94 -0.95 -0.9 -1.12 -0.88 -0.95 ...
##  $ PPARd    : num  -1.51 -1.59 -1.71 -1.57 -1.53 -1.56 -1.49 -1.57 -1.58 -1.54 ...
##  $ PPARg    : num  -1.06 -1.02 -1.14 -1.05 -1.09 -1.01 -1 -1.13 -0.97 -1.07 ...
##  $ PXR      : num  -0.99 -0.96 -1.1 -0.99 -1 -1.03 -0.93 -1.07 -0.98 -0.96 ...
##  $ Pex11a   : num  -1 -1.02 -1.2 -1 -0.95 -1.07 -1.05 -1.02 -1 -1.01 ...
##  $ RARa     : num  -1.2 -1.06 -1.16 -1.17 -1.15 -1.13 -1.09 -1.24 -1.03 -1.09 ...
##  $ RARb2    : num  -1.19 -1.11 -1.23 -1.16 -1.14 -1.07 -1.09 -1.18 -1.12 -1.1 ...
```

```
##  $ RXRa     : num  -0.67 -0.59 -0.68 -0.72 -0.78 -0.62 -0.65 -0.76 -0.55 -0.67 ...
##  $ RXRb2    : num  -0.95 -0.95 -1.07 -0.95 -0.98 -0.94 -0.92 -1.03 -0.94 -0.95 ...
##  $ RXRg1    : num  -1.16 -1.1 -1.21 -1.1 -1.11 -1.03 -1.07 -1.19 -1.05 -1.04 ...
##  $ S14      : num  -0.93 -0.86 -0.84 -1.05 -0.65 -0.4 -0.73 -0.62 -0.99 -0.25 ...
##  $ SHP1     : num  -1.1 -0.97 -1.09 -1.03 -1.13 -0.98 -0.95 -1.21 -0.93 -0.97 ...
##  $ SIAT4c   : num  -1.07 -0.97 -1.04 -0.99 -0.94 -0.93 -0.89 -1.04 -0.93 -0.95 ...
##  $ SPI1.1   : num  1.19 1.15 1.09 1.07 1.22 1.05 1.15 1.18 1.21 1.04 ...
##  $ SR.BI    : num  -0.84 -0.86 -0.95 -0.95 -1.06 -0.8 -0.83 -1 -0.83 -0.77 ...
##  $ THB      : num  -0.79 -0.85 -0.92 -0.79 -0.84 -0.86 -0.8 -0.86 -0.83 -0.85 ...
##  $ THIOL    : num  -0.18 -0.15 -0.24 -0.15 -0.35 -0.29 -0.22 -0.23 -0.17 -0.18 ...
##  $ TRa      : num  -1.48 -1.46 -1.58 -1.54 -1.46 -1.44 -1.32 -1.56 -1.46 -1.35 ...
##  $ TRb      : num  -1.07 -1 -1.16 -1.11 -1.01 -1 -0.97 -1.08 -1.02 -0.98 ...
##  $ Tpalpha  : num  -0.69 -0.74 -0.81 -0.74 -0.82 -0.76 -0.72 -0.76 -0.65 -0.83 ...
##  $ Tpbeta   : num  -1.11 -1.09 -1.14 -1.04 -1.2 -1.05 -1 -1.16 -0.91 -1.07 ...
##   [list output truncated]
```

```
## check if there are missing values
any(is.na(nutrimouse$gene))
```

```
## [1] FALSE
```

```
## investigate each variable
summary(nutrimouse$gene[, 1])
```

```
##    Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
## -0.5800 -0.5025 -0.4600 -0.4552 -0.4200 -0.3000
```

```
colors <- rainbow(20, alpha=1)
plot(density(scale(nutrimouse$gene[, 1], center=T, scale=F)),
     col=colors[1], xlim=c(-0.5,0.5), ylim=c(0,8))
sapply(2:20, function(i) {
    lines(density(scale(nutrimouse$gene[, i], center=T, scale=F)), col=colors[i])
})
```

```
## [[1]]
## NULL
##
## [[2]]
## NULL
##
## [[3]]
## NULL
##
## [[4]]
## NULL
##
## [[5]]
## NULL
##
## [[6]]
## NULL
##
## [[7]]
## NULL
##
## [[8]]
```

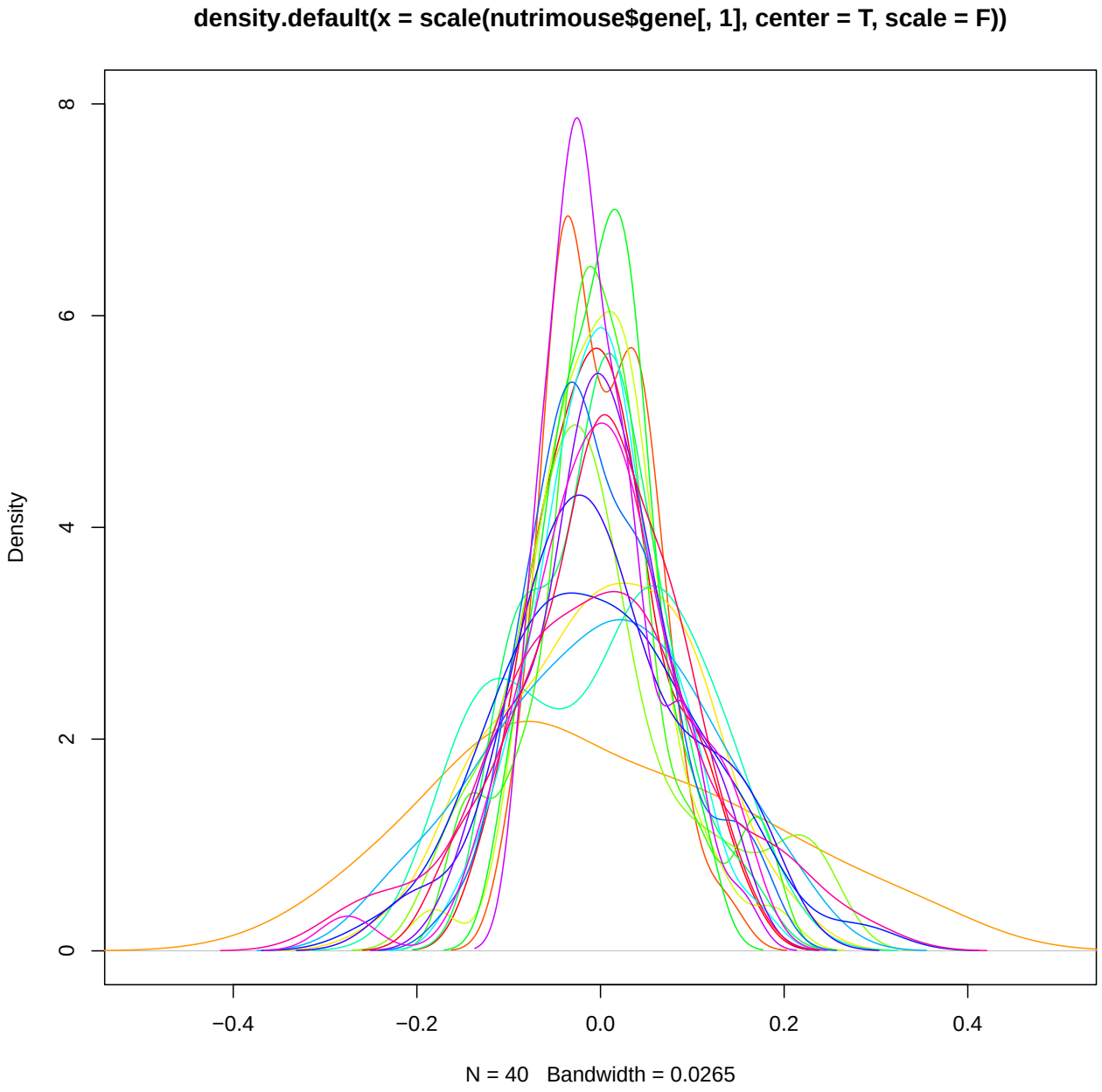
```
## NULL
##
## [[9]]
## NULL
##
## [[10]]
## NULL
##
## [[11]]
## NULL
##
## [[12]]
## NULL
##
## [[13]]
## NULL
##
## [[14]]
## NULL
##
## [[15]]
## NULL
##
## [[16]]
## NULL
##
## [[17]]
## NULL
##
## [[18]]
## NULL
##
## [[19]]
## NULL
```

```
apply(nutrimouse$gene, 2, summary)
```

```
##            X36b4    ACAT1    ACAT2     ACBP    ACC1    ACC2    ACOTH    ADISP
## Min.    -0.58000 -0.75000 -1.10000 -0.66000 -1.4400 -1.2000 -1.06000 -1.08000
## 1st Qu. -0.50250 -0.69000 -0.88000 -0.50250 -1.3000 -1.0900 -0.95000 -1.02000
## Median  -0.46000 -0.66000 -0.79500 -0.42500 -1.2600 -1.0450 -0.92000 -0.97000
## Mean    -0.45525 -0.65525 -0.76675 -0.43375 -1.2585 -1.0280 -0.91075 -0.97825
## 3rd Qu. -0.42000 -0.62000 -0.64500 -0.35500 -1.2200 -0.9875 -0.88000 -0.94000
## Max.    -0.30000 -0.52000 -0.39000 -0.24000 -1.0700 -0.7900 -0.73000 -0.87000
##            ADSS1   ALDH3   AM2R     AOX     BACT     BIEN    BSEP    Bcl.3
## Min.    -1.19000 -0.9900 -0.780 -0.4800 -0.44000 -1.16000 -0.9000 -1.22000
## 1st Qu. -1.14000 -0.9100 -0.670 -0.3175 -0.32250 -0.99000 -0.7600 -1.10250
## Median  -1.07500 -0.7850 -0.630 -0.2300 -0.30000 -0.92000 -0.7000 -1.06500
## Mean    -1.07575 -0.8100 -0.628 -0.2505 -0.28275 -0.92125 -0.6910 -1.05875
## 3rd Qu. -1.03500 -0.7475 -0.590 -0.1675 -0.23500 -0.85500 -0.6275 -1.01000
## Max.    -0.91000 -0.6200 -0.460 -0.0400 -0.11000 -0.64000 -0.5100 -0.91000
##           C16SR    CACP    CAR1     CBS   CIDEA     COX1   COX2    CPT2   CYP24
## Min.    1.55000 -1.2600 -1.1900 -0.5600 -1.3300 -1.18000 -1.280 -1.2000 -1.3700
## 1st Qu. 1.59000 -1.0325 -0.9900 -0.4450 -1.2325 -1.09250 -1.180 -1.0100 -1.2600
## Median  1.61000 -0.9800 -0.9100 -0.4000 -1.1700 -1.05500 -1.130 -0.9450 -1.1800
```

```
## Mean    1.62675 -0.9845 -0.9135 -0.3995 -1.1840 -1.04975 -1.135 -0.9565 -1.1925
## 3rd Qu. 1.65250 -0.9375 -0.8475 -0.3375 -1.1400 -1.01000 -1.090 -0.8800 -1.1375
## Max.    1.78000 -0.8300 -0.6300 -0.2600 -1.0700 -0.88000 -1.040 -0.8200 -1.0500
##           CYP26  CYP27a1 CYP27b1  CYP2b10  CYP2b13  CYP2c29  CYP3A11  CYP4A10
## Min.    -1.3200 -0.88000  -1.350 -1.32000 -1.37000 -0.52000 -1.02000 -1.33000
## 1st Qu. -1.2225 -0.78500  -1.245 -1.23000 -1.19250 -0.28250 -0.71250 -1.15250
## Median  -1.1500 -0.73000  -1.180 -1.20000 -1.14000 -0.14000 -0.53000 -1.05000
## Mean    -1.1560 -0.72725  -1.200 -1.18475 -1.14575 -0.14725 -0.50825 -0.97975
## 3rd Qu. -1.1000 -0.67000  -1.150 -1.15000 -1.09750 -0.03000 -0.38500 -0.81750
## Max.    -0.9600 -0.59000  -0.990 -1.04000 -0.96000  0.18000  0.06000 -0.48000
##         CYP4A14   CYP7a   CYP8b1      FAS     FAT     FDFT     FXR    G6PDH
## Min.    -1.2900 -0.9300 -1.01000 -1.05000 -1.0900 -1.17000 -1.0600 -1.30000
## 1st Qu. -1.1500 -0.8000 -0.76000 -0.67000 -1.0400 -1.02000 -0.9525 -1.20250
## Median  -1.0800 -0.7700 -0.67000 -0.49000 -0.9950 -0.99000 -0.9000 -1.15000
## Mean    -0.9930 -0.7695 -0.68225 -0.45175 -0.9910 -0.98075 -0.9105 -1.15125
## 3rd Qu. -0.8925 -0.7400 -0.59000 -0.22500 -0.9475 -0.93750 -0.8775 -1.10750
## Max.    -0.1500 -0.6100 -0.50000  0.18000 -0.7500 -0.81000 -0.7600 -0.96000
##           G6Pase      GK      GS    GSTa  GSTmu  GSTpi2 HMGCoAred    HPNCL
## Min.    -1.06000 -0.9600 -1.3800 -0.4300 -0.440 0.00000   -1.0700 -0.97000
## 1st Qu. -0.82000 -0.8000 -1.3025 -0.1525 -0.200 0.12000   -0.9700 -0.75000
## Median  -0.69000 -0.7000 -1.2250 -0.0900 -0.140 0.21000   -0.9300 -0.69000
## Mean    -0.69825 -0.7145 -1.2325 -0.1030 -0.119 0.22975   -0.9135 -0.69375
## 3rd Qu. -0.53500 -0.6200 -1.1675 -0.0350 -0.050 0.33250   -0.8750 -0.60750
## Max.    -0.38000 -0.4600 -1.1200  0.0400  0.230 0.55000   -0.7000 -0.53000
##            IL.2  L.FABP      LCE    LDLr    LPK      LPL    LXRa    LXRb
## Min.    -1.1600 -0.4600 -0.26000 -0.9600 -0.570 -1.11000 -0.9100 -1.1600
## 1st Qu. -1.0025 -0.0750 -0.10000 -0.8525 -0.395 -1.03000 -0.8400 -1.0225
## Median  -0.9450  0.0600 -0.06000 -0.8200 -0.350 -0.99000 -0.8150 -0.9900
## Mean    -0.9505  0.0340 -0.05275 -0.8195 -0.344 -0.99075 -0.8115 -0.9960
## 3rd Qu. -0.8975  0.1825  0.00000 -0.7675 -0.295 -0.95000 -0.7775 -0.9675
## Max.    -0.8200  0.2800  0.12000 -0.6800 -0.130 -0.86000 -0.6500 -0.8400
##             Lpin    Lpin1  Lpin2   Lpin3   M.CPT1    MCAD     MDR1     MDR2
## Min.    -1.13000 -1.10000 -1.140 -1.2900 -1.29000 -0.7300 -1.30000 -0.92000
## 1st Qu. -0.85500 -0.87000 -0.910 -1.1975 -1.16500 -0.6600 -1.16250 -0.83000
## Median  -0.72500 -0.76000 -0.855 -1.1450 -1.12000 -0.6200 -1.12000 -0.78000
## Mean    -0.75325 -0.76475 -0.849 -1.1475 -1.12575 -0.6050 -1.13425 -0.77875
## 3rd Qu. -0.61500 -0.64000 -0.775 -1.0975 -1.09000 -0.5575 -1.09000 -0.71750
## Max.    -0.48000 -0.49000 -0.670 -0.9800 -0.96000 -0.4200 -0.99000 -0.65000
##             MRP6       MS   MTHFR    NGFiB    NURR1    Ntcp    OCTN2     PAL
## Min.    -1.09000 -1.20000 -1.1000 -1.29000 -1.32000 -0.6500 -1.28000 -1.3200
## 1st Qu. -1.00250 -1.11000 -1.0025 -1.20000 -1.21000 -0.4925 -1.19000 -1.2550
## Median  -0.95500 -1.06500 -0.9700 -1.12000 -1.14000 -0.4400 -1.15000 -1.2000
## Mean    -0.94775 -1.06075 -0.9720 -1.12925 -1.16125 -0.4370 -1.13925 -1.1445
## 3rd Qu. -0.87750 -1.00750 -0.9300 -1.07750 -1.10750 -0.3675 -1.08000 -1.0075
## Max.    -0.83000 -0.88000 -0.8800 -0.91000 -0.95000 -0.2500 -1.04000 -0.8900
##             PDK4     PECI     PLTP    PMDCI     PON   PPARa   PPARd  PPARg
## Min.    -1.28000 -1.11000 -1.15000 -1.07000 -0.7100 -1.1400 -1.7100 -1.190
## 1st Qu. -1.17250 -0.92250 -1.09250 -0.94250 -0.6325 -1.0225 -1.5900 -1.090
## Median  -1.13000 -0.84000 -1.05000 -0.76500 -0.5800 -0.9500 -1.5600 -1.055
## Mean    -1.13525 -0.84725 -1.03625 -0.76725 -0.5825 -0.9660 -1.5595 -1.052
## 3rd Qu. -1.08000 -0.79750 -0.99750 -0.60000 -0.5375 -0.9000 -1.5100 -1.010
## Max.    -1.01000 -0.58000 -0.85000 -0.44000 -0.4500 -0.8300 -1.4300 -0.900
##              PXR  Pex11a     RARa   RARb2    RXRa  RXRb2   RXRg1      S14
## Min.    -1.13000 -1.2000 -1.30000 -1.3000 -0.7800 -1.070 -1.2300 -1.05000
```

```
## 1st Qu. -1.03000 -1.0500 -1.18250 -1.1900 -0.6725 -1.000 -1.1425 -0.98000
## Median  -0.99000 -1.0200 -1.13000 -1.1350 -0.6350 -0.960 -1.1000 -0.85500
## Mean    -0.99225 -1.0220 -1.13325 -1.1445 -0.6360 -0.964 -1.0955 -0.80675
## 3rd Qu. -0.94750 -0.9875 -1.07500 -1.0900 -0.5875 -0.935 -1.0500 -0.65750
## Max.    -0.84000 -0.9000 -0.97000 -0.9900 -0.4900 -0.780 -0.9000 -0.25000
##             SHP1   SIAT4c  SPI1.1  SR.BI     THB  THIOL    TRa      TRb
## Min.    -1.21000 -1.16000 0.96000 -1.060 -0.9200 -0.900 -1.670 -1.22000
## 1st Qu. -1.07500 -0.99000 1.03750 -0.920 -0.8500 -0.590 -1.510 -1.11000
## Median  -0.99000 -0.96000 1.07500 -0.830 -0.8200 -0.345 -1.460 -1.06000
## Mean    -1.00675 -0.96225 1.09075 -0.843 -0.8170 -0.411 -1.457 -1.05425
## 3rd Qu. -0.94750 -0.92750 1.15000 -0.800 -0.7875 -0.230 -1.395 -0.99750
## Max.    -0.78000 -0.84000 1.23000 -0.610 -0.6900 -0.030 -1.220 -0.92000
##          Tpalpha Tpbeta    UCP2     UCP3      VDR    VLDLr    Waf1     ap2
## Min.    -1.00000 -1.310 -1.0800 -1.27000 -1.30000 -1.19000 -1.3000 -1.3700
## 1st Qu. -0.86000 -1.200 -1.0025 -1.15250 -1.18000 -1.09250 -1.1500 -1.2225
## Median  -0.83000 -1.140 -0.9800 -1.11000 -1.12000 -1.05500 -1.1300 -1.1900
## Mean    -0.81825 -1.130 -0.9660 -1.10775 -1.13175 -1.05325 -1.1235 -1.1880
## 3rd Qu. -0.76000 -1.065 -0.9275 -1.05000 -1.08000 -1.01000 -1.0875 -1.1475
## Max.    -0.65000 -0.910 -0.7600 -0.92000 -0.94000 -0.91000 -0.9400 -1.0800
##         apoA.I    apoB    apoC3    apoE    c.fos cHMGCoAS   cMOAT  eif2g
## Min.    0.5400 -0.2700 -0.49000 0.86000 -1.22000 -1.24000 -1.0200 -1.230
## 1st Qu. 0.6575 -0.2000 -0.39000 0.98000 -1.15000 -1.10250 -0.8950 -1.100
## Median  0.7200 -0.1700 -0.34000 1.04000 -1.11000 -1.03000 -0.8700 -1.055
## Mean    0.7295 -0.1675 -0.34075 1.02825 -1.10525 -1.01375 -0.8485 -1.058
## 3rd Qu. 0.8100 -0.1450 -0.30000 1.07000 -1.06000 -0.91000 -0.7875 -1.020
## Max.    0.9200  0.0100 -0.18000 1.18000 -0.98000 -0.78000 -0.6900 -0.840
##            hABC1  i.BABP    i.BAT i.FABP   i.NOS   mABC1 mHMGCoAS
## Min.    -1.25000 -0.8900 -1.89000 -1.300 -1.4300 -0.9800  -0.5800
## 1st Qu. -1.17250 -0.8325 -1.74250 -1.170 -1.2850 -0.9200  -0.3000
## Median  -1.13500 -0.8000 -1.69000 -1.140 -1.2400 -0.8700  -0.2100
## Mean    -1.13825 -0.7935 -1.69775 -1.122 -1.2460 -0.8765  -0.2210
## 3rd Qu. -1.09750 -0.7475 -1.66000 -1.075 -1.2075 -0.8375  -0.1275
## Max.    -0.98000 -0.6700 -1.55000 -0.930 -1.0900 -0.8000   0.0600
```



3. Perform PCA and investigate variances, sample distribution and variable relationship with plots. A number of methods in different R packages can perform PCA, e.g. `stats::prcomp`, `stats::princomp`, `mixOmics::pca`, `multiblock::pca`, `psych::principal`, `FactoMineR::PCA`, etc.

```
pca.res <- prcomp(nutrimouse$gene, center=TRUE, scale.=F)
names(pca.res)
```

```
## [1] "sdev"     "rotation" "center"   "scale"    "x"
```

```
summary(pca.res)
```

```
## Importance of components:
##                           PC1    PC2    PC3     PC4     PC5     PC6     PC7
## Standard deviation     0.6763 0.5064 0.4033 0.28206 0.24164 0.19445 0.17513
## Proportion of Variance 0.3497 0.1961 0.1244 0.06084 0.04465 0.02891 0.02345
```

```
## Cumulative Proportion  0.3497 0.5458 0.6702 0.73107 0.77572 0.80463 0.82808
##                            PC8     PC9    PC10    PC11    PC12    PC13    PC14
## Standard deviation     0.16498 0.14796 0.13623 0.13425 0.11505 0.11208 0.11052
## Proportion of Variance 0.02081 0.01674 0.01419 0.01378 0.01012 0.00961 0.00934
## Cumulative Proportion  0.84889 0.86563 0.87983 0.89361 0.90373 0.91333 0.92267
##                           PC15    PC16    PC17    PC18    PC19    PC20    PC21
## Standard deviation     0.10450 0.09952 0.09052 0.08962 0.07914 0.07511 0.07313
## Proportion of Variance 0.00835 0.00757 0.00627 0.00614 0.00479 0.00431 0.00409
## Cumulative Proportion  0.93102 0.93860 0.94486 0.95101 0.95579 0.96011 0.96420
##                           PC22    PC23    PC24    PC25    PC26    PC27    PC28
## Standard deviation     0.06913 0.06708 0.06308 0.06186 0.06029 0.05810 0.05639
## Proportion of Variance 0.00365 0.00344 0.00304 0.00293 0.00278 0.00258 0.00243
## Cumulative Proportion  0.96785 0.97129 0.97434 0.97726 0.98004 0.98262 0.98505
##                           PC29    PC30    PC31    PC32    PC33    PC34    PC35
## Standard deviation     0.05151 0.04984 0.04840 0.04724 0.04602 0.04083 0.03979
## Proportion of Variance 0.00203 0.00190 0.00179 0.00171 0.00162 0.00127 0.00121
## Cumulative Proportion  0.98708 0.98898 0.99077 0.99248 0.99410 0.99538 0.99659
##                           PC36    PC37    PC38    PC39      PC40
## Standard deviation     0.03680 0.03468 0.03282 0.02883 1.858e-15
## Proportion of Variance 0.00104 0.00092 0.00082 0.00064 0.000e+00
## Cumulative Proportion  0.99762 0.99854 0.99936 1.00000 1.000e+00
```

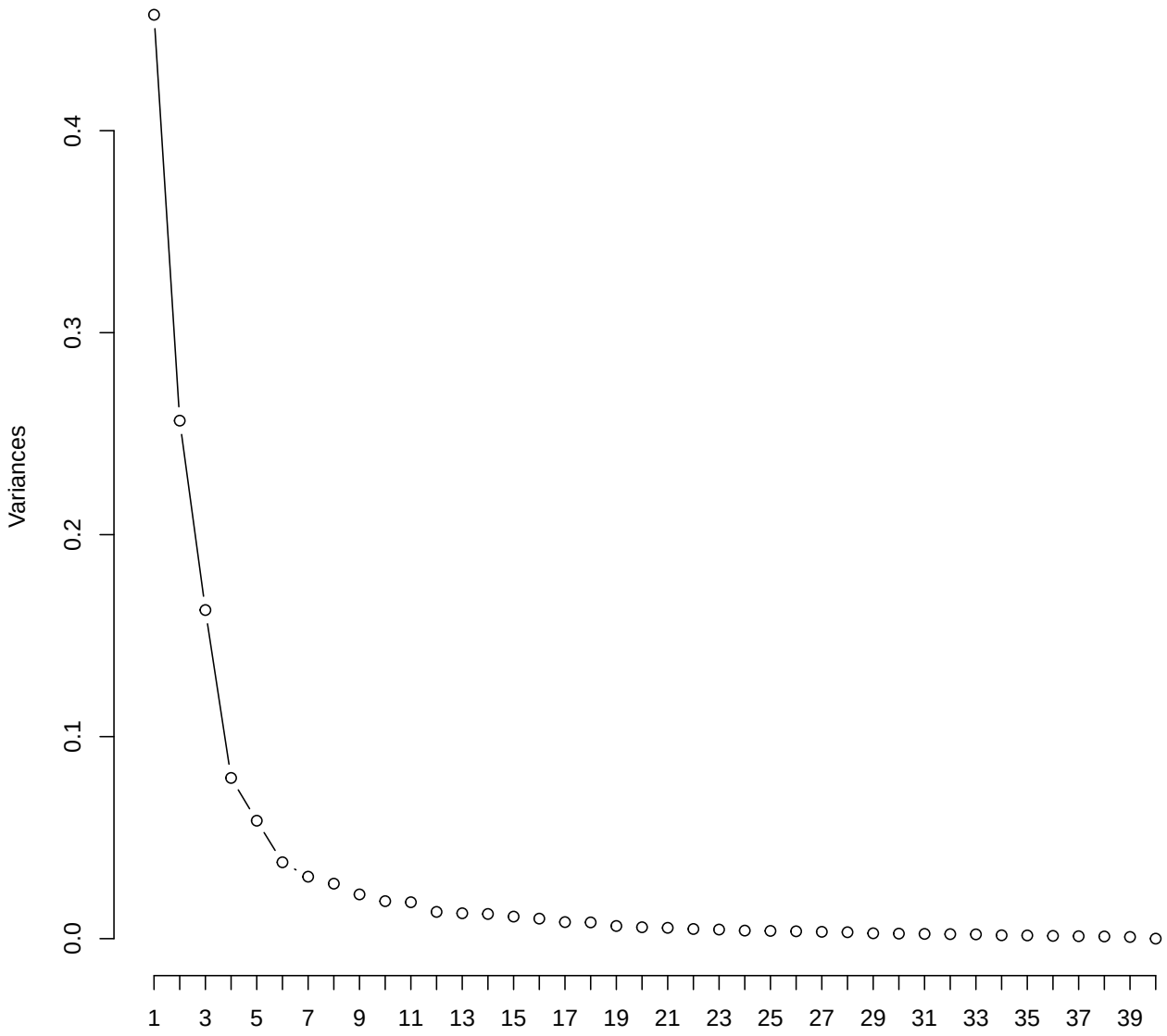
Variances = eigenvalues of the covariance matrix = (standard deviation)^2

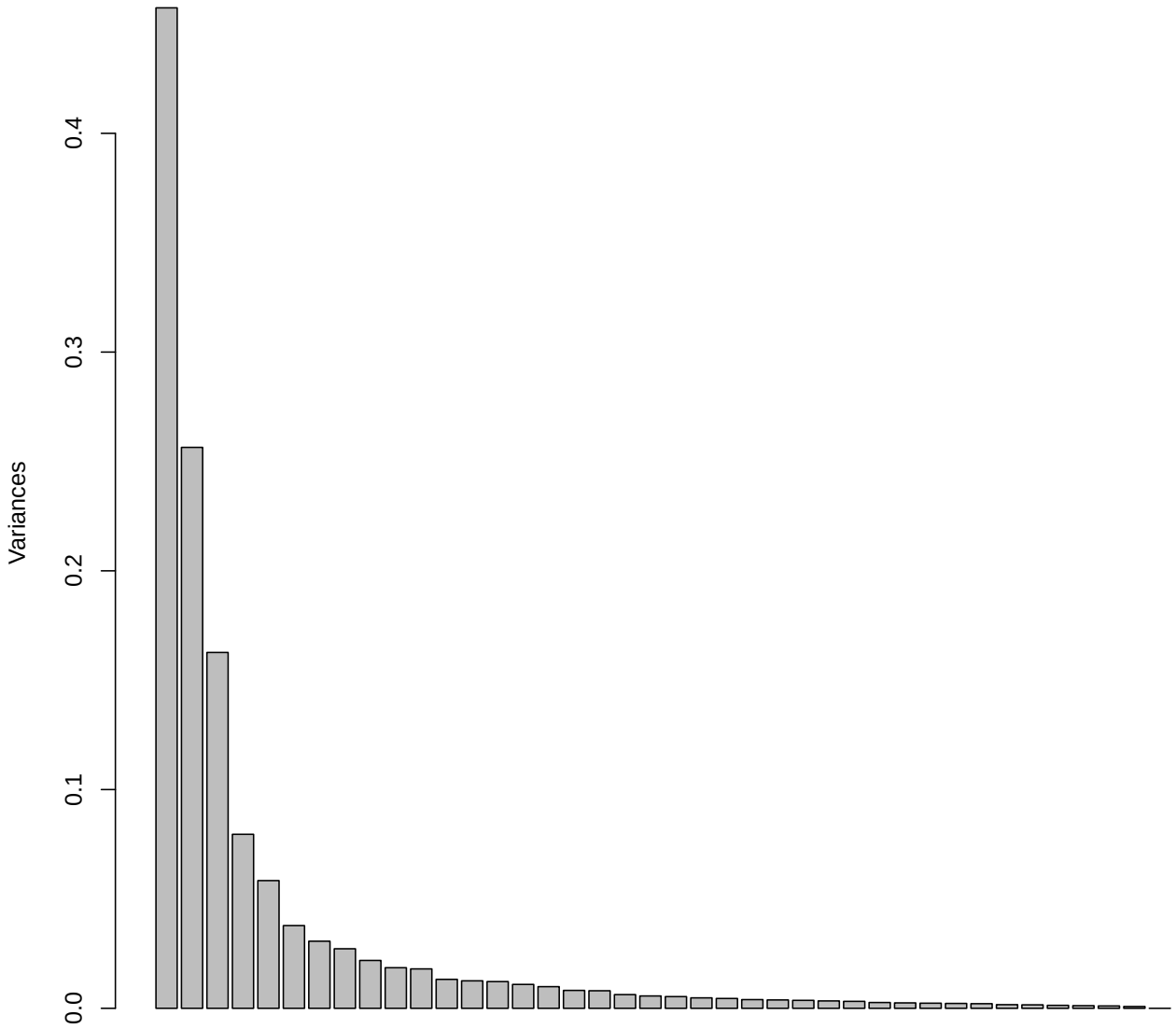
```
variances <- pca.res$sdev^2
variances
```

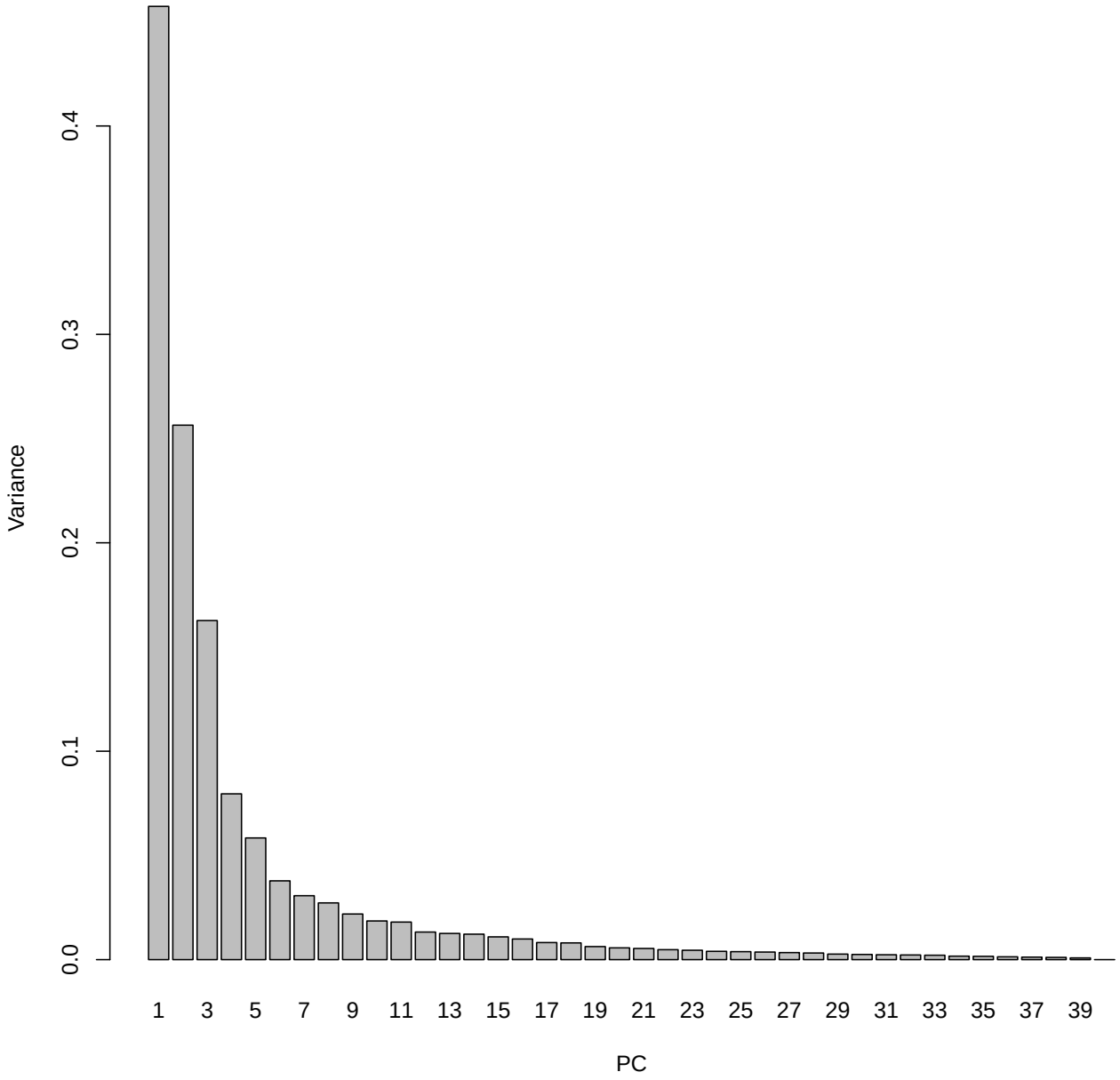
```
##  [1] 4.573742e-01 2.564410e-01 1.626804e-01 7.955690e-02 5.838751e-02
##  [6] 3.780991e-02 3.066913e-02 2.721979e-02 2.189256e-02 1.855921e-02
## [11] 1.802243e-02 1.323667e-02 1.256153e-02 1.221509e-02 1.091924e-02
## [16] 9.905054e-03 8.193579e-03 8.032182e-03 6.262595e-03 5.641794e-03
## [21] 5.348430e-03 4.779376e-03 4.500169e-03 3.978795e-03 3.826089e-03
## [26] 3.634453e-03 3.376009e-03 3.179730e-03 2.653212e-03 2.484088e-03
## [31] 2.342963e-03 2.231208e-03 2.117845e-03 1.667351e-03 1.583188e-03
## [36] 1.353925e-03 1.202714e-03 1.076873e-03 8.311648e-04 3.452555e-30
```

Scree plot: plot of variances.

```
screeplot(pca.res, npcs=length(variances), type='lines')
screeplot(pca.res, npcs=length(variances), type='barplot')
barplot(variances, xlab='PC', ylab='Variance', names.arg=1:length(variances))
```

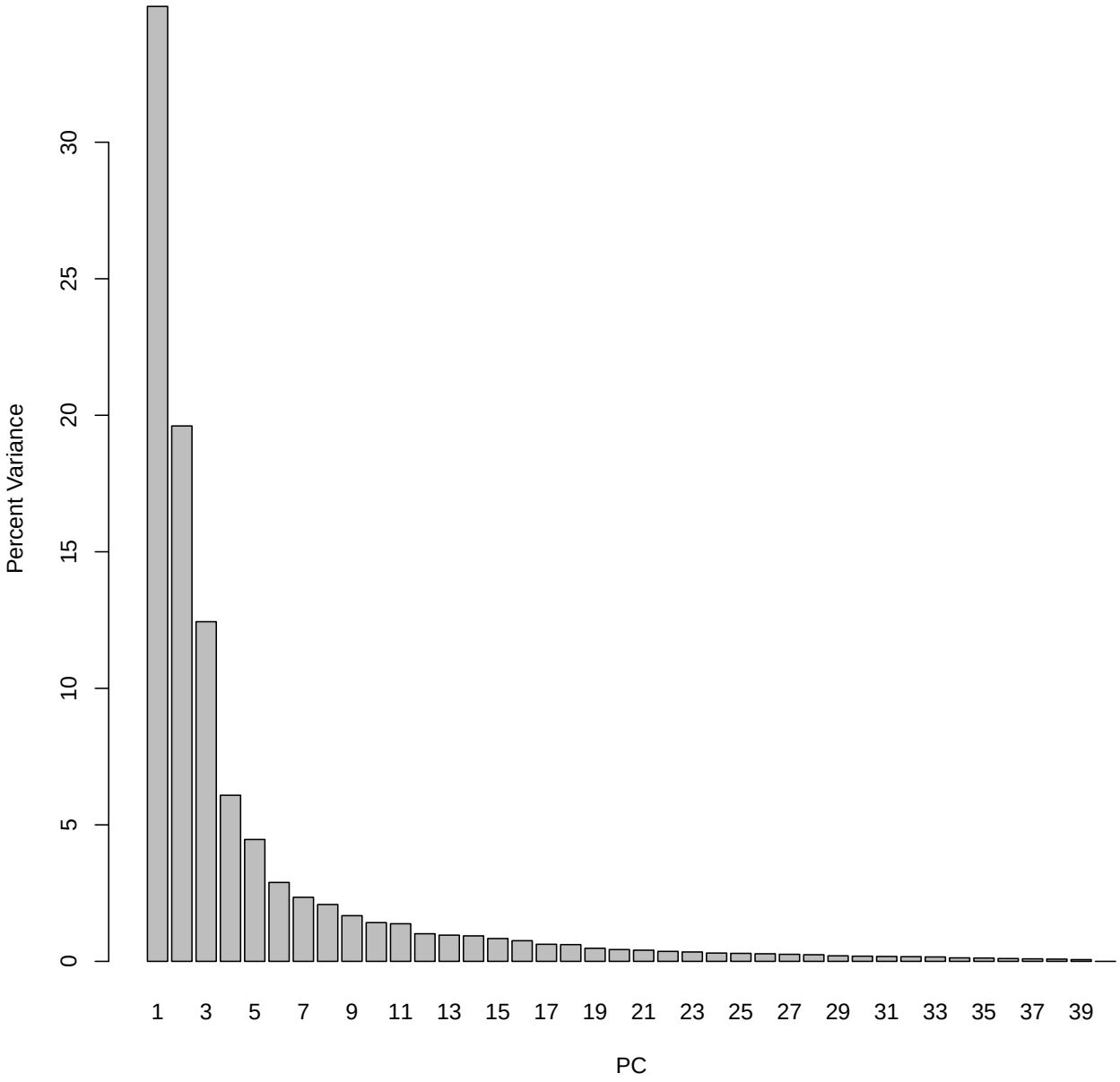

pca.res
Variances
0.0
0.1
0.2
0.3
0.4
1
3
5
7
9
11
13
15
17
19
21
23
25
27
29
31
33
35
37
39


pca.res
Variances
0.0
0.1
0.2
0.3
0.4



Scree plot on variance percentage.

```
varPercent <- variances/sum(variances) * 100
barplot(varPercent, xlab='PC', ylab='Percent Variance', names.arg=1:length(varPercent))
```



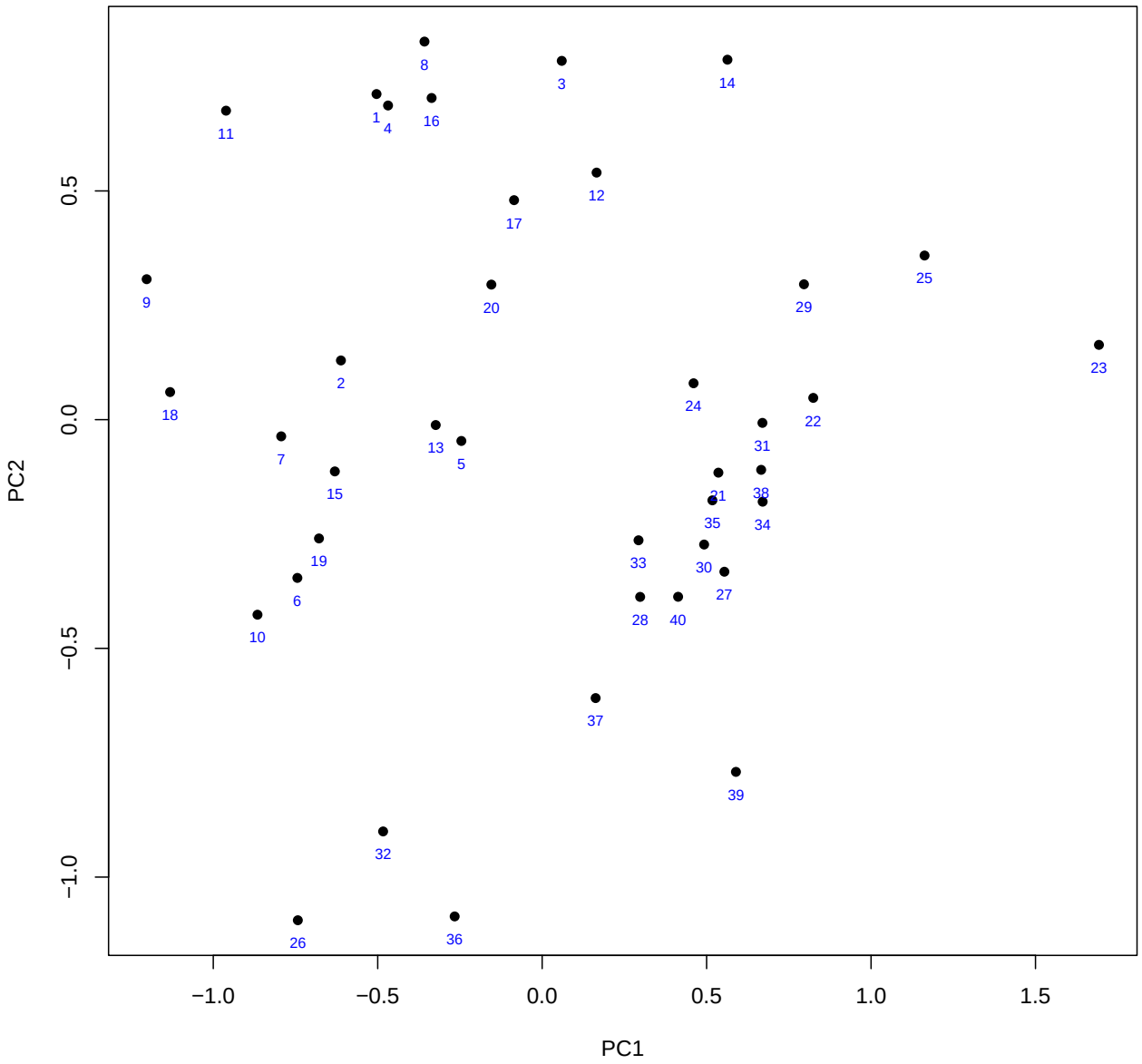
Scores: sample coordinates in the new reference (rotated axes or principal components).

```
scores <- pca.res$x
str(scores)
```

```
##  num [1:40, 1:40] -0.5036 -0.6119 0.0596 -0.4686 -0.2457 ...
##  - attr(*, "dimnames")=List of 2
##   ..$ : chr [1:40] "1" "2" "3" "4" ...
##   ..$ : chr [1:40] "PC1" "PC2" "PC3" "PC4" ...
```

Score plot: plot of sample distribution.

```
PCx <- "PC1"
PCy <- "PC2"
plot(scores[, PCx], scores[, PCy], xlab=PCx, ylab=PCy, pch=16)
text(scores[, PCx], scores[, PCy]-0.05, rownames(scores), col='blue', cex=0.7)
```



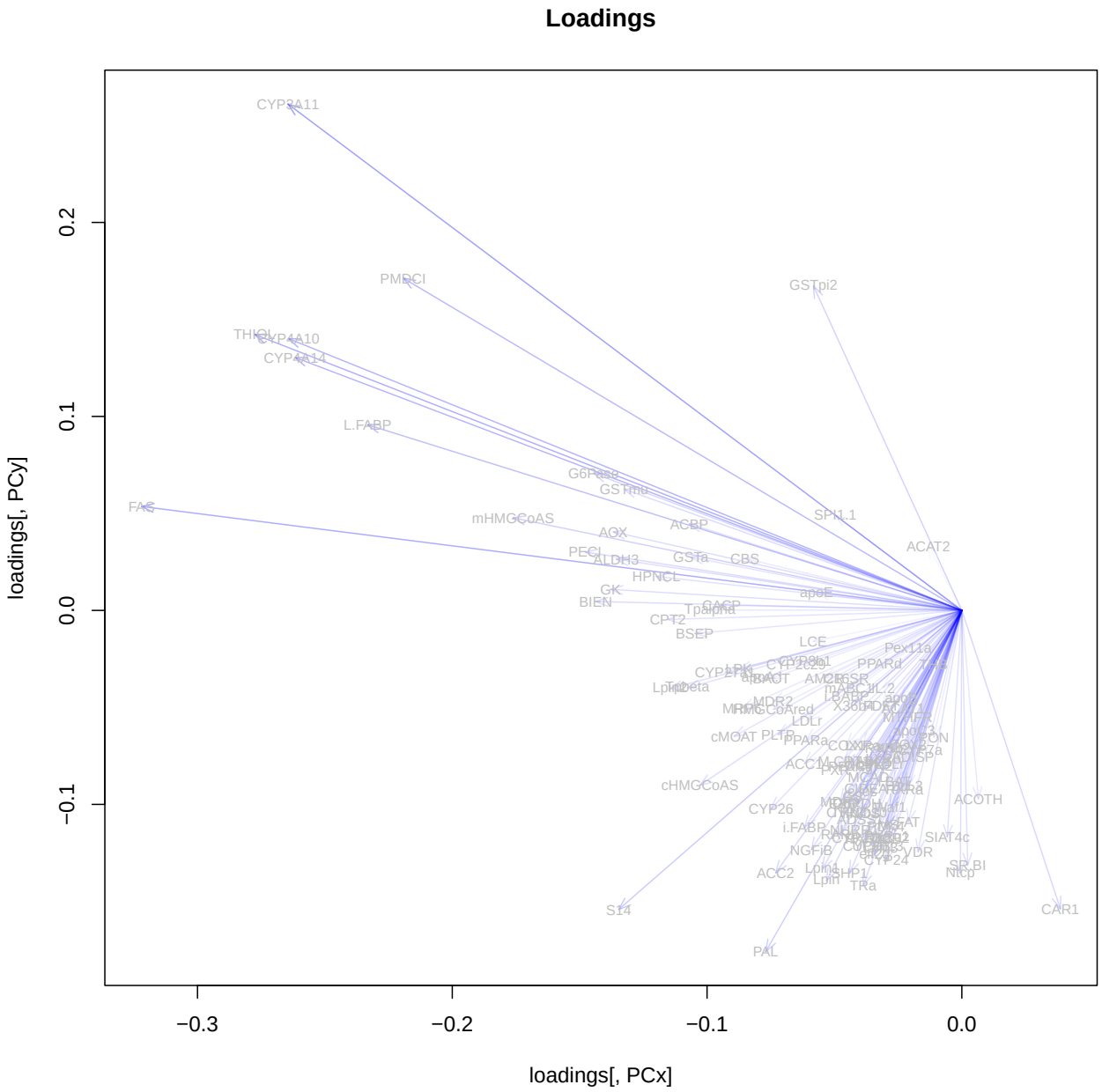
Loadings: contributions of variables to principal components (eigenvectors of covariance matrix).

```
loadings <- pca.res$rotation
str(loadings)
```

```
##  num [1:120, 1:40] -0.0425 -0.023 -0.0131 -0.107 -0.0618 ...
##  - attr(*, "dimnames")=List of 2
##   ..$ : chr [1:120] "X36b4" "ACAT1" "ACAT2" "ACBP" ...
##   ..$ : chr [1:40] "PC1" "PC2" "PC3" "PC4" ...
```

Loading plot: plot of variables' contribution, revealing their relationship.

```
plot(loadings[, PCx], loadings[, PCy], type='n', main="Loadings")
arrows(0, 0, loadings[, PCx], loadings[, PCy], xlab=PCx, ylab=PCy,
       length=0.1, angle=20, col=rgb(0,0,1,alpha=apply(loadings[, c(PCx, PCy)], 1, norm, "2")))
text(loadings[, PCx], loadings[, PCy], rownames(loadings), col='grey', cex=0.7)
```

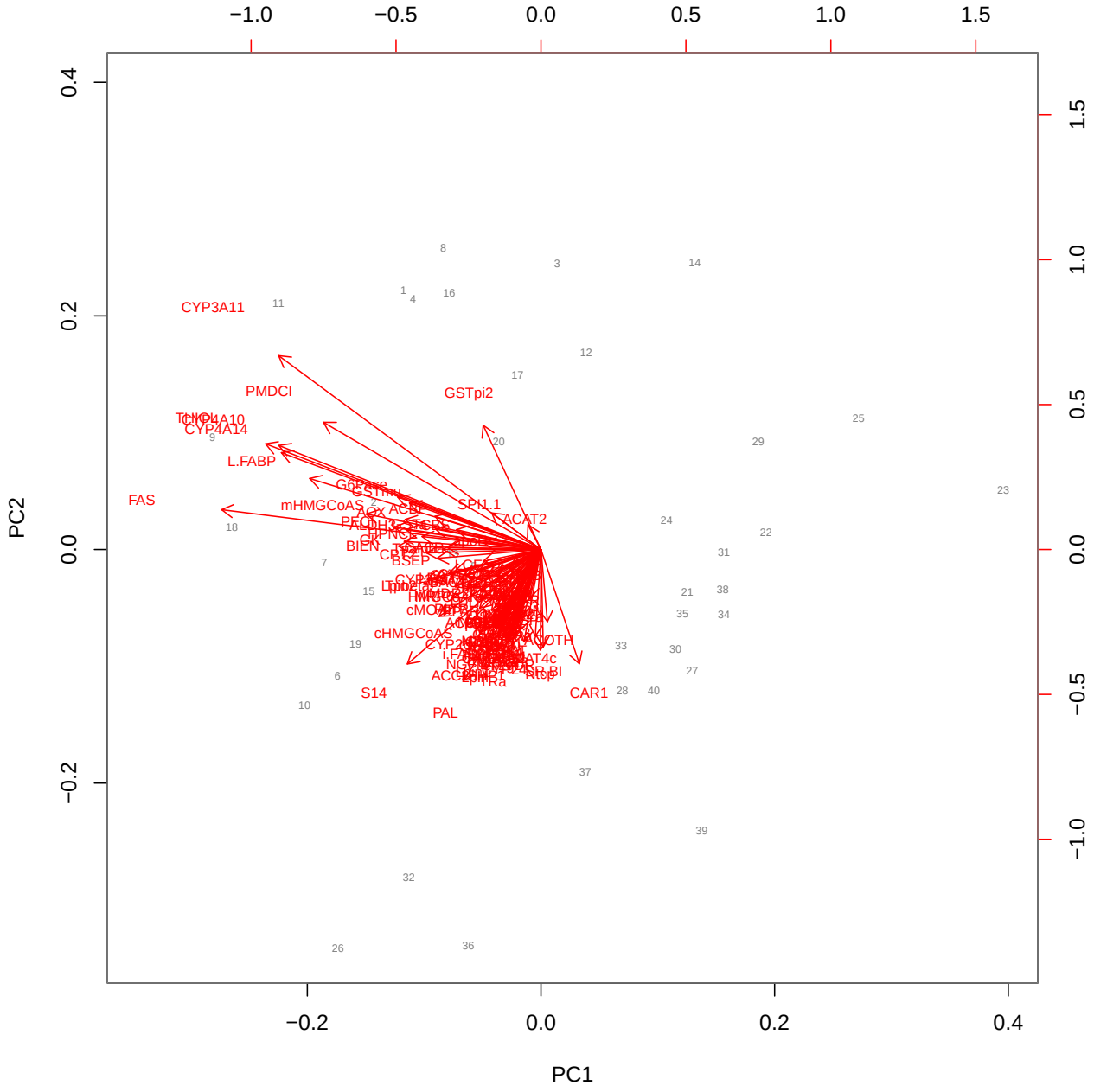


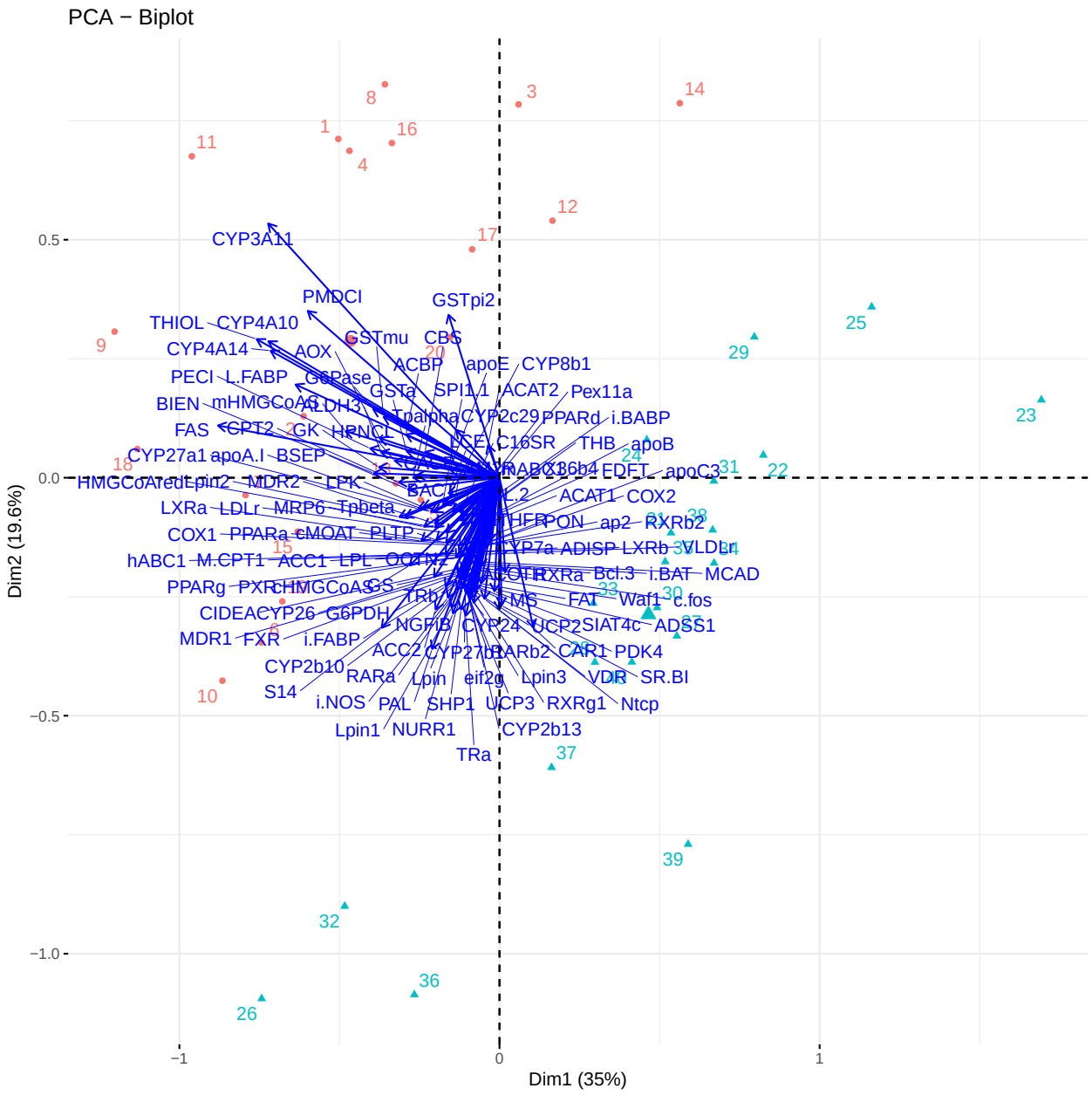
Both score and loading plot can be plot altogether with the `biplot` function.

```
## biplot
biplot(pca.res, expand=1, cex=c(0.5, 0.7), col=c("gray50", "red"))

# fviz_pca_var(pca.res, col.var = "contrib", # Color by contributions to the PC
#              gradient.cols = c("white", "red"),#c("#00AFBB", "#E7B800", "#FC4E07"),
#              repel = T)
library(factoextra)
fviz_pca_biplot(pca.res, repel = TRUE,
                col.var = "blue", # Variables color
                #col.ind = "gray50"  # Individuals color
                habillage = nutrimouse$genotype,
                addEllipses = F,
                legend="none"
```

)

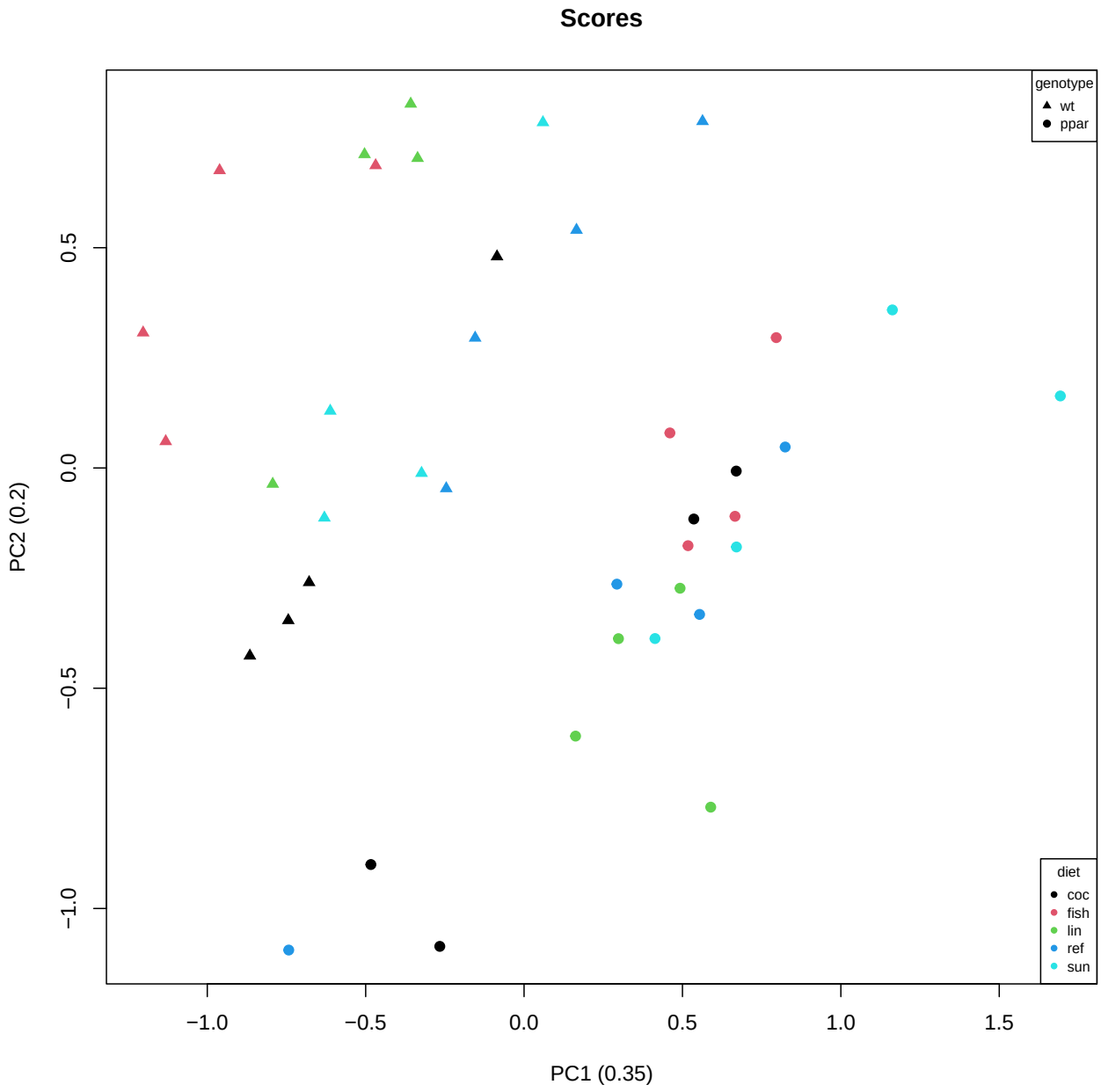

−1.0
−0.5
0.0
0.5
1.0
1.5
0.4
0.2
0.0
−0.2
PC2
PC1
1.5
1.0
0.5
0.0
−0.5
−1.0
CYP3A11
PMDCI
GSTpi2
CYP4A10
CYP4A14
L.FABP
FAS
mHMGCoAS
SPI1.1
ACAT2
BSEP
cHMGCoAS
S14
PAL
CAR1



4. Visually investigate the sample distribution with coloring by metadata or expression of certain genes. The samples can be colored with some metadata, e.g *genotype* or *diet*,

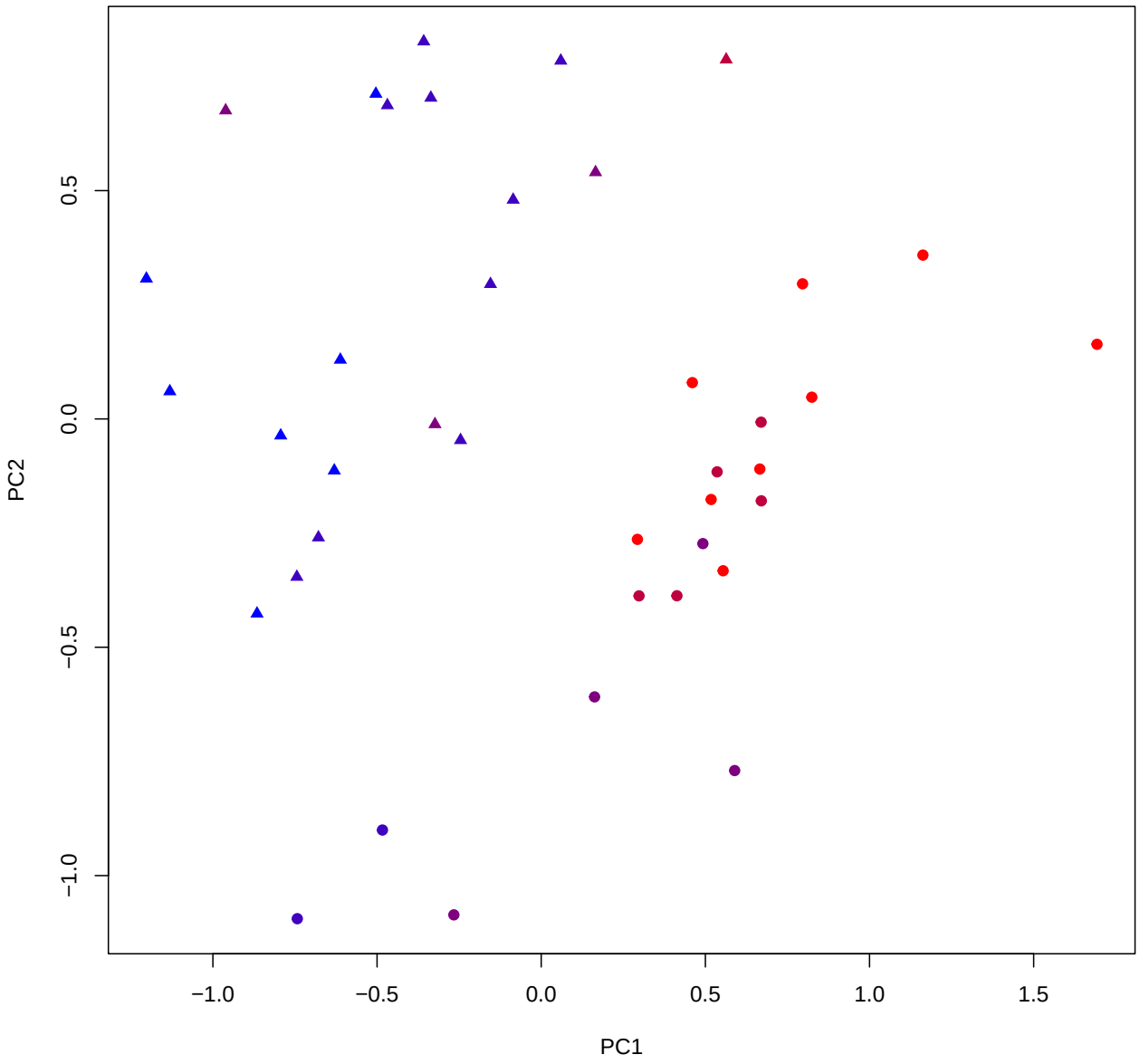
```
plot(scores[, PCx], scores[, PCy], main="Scores",
     col=c(1:nlevels(nutrimouse$diet))[nutrimouse$diet],
     pch=c(17,19)[nutrimouse$genotype],
     xlab=paste0(PCx,
                 " (",
                 round((summary(pca.res)$importance)[2, PCx], 2), ")"),
     ylab=paste0(PCy,
                 " (",
                 round((summary(pca.res)$importance)[2, PCy], 2), ")")
)
legend("topright", title="genotype",
```

```
       legend=levels(nutrimouse$genotype),
       pch=c(17,19), cex=0.7)
legend("bottomright", title="diet",
       legend=levels(nutrimouse$diet),
       col=c(1:5), cex=0.7, pch=16)
```



or by some gene expression.

```
nbreaks <- 5
plot(scores[, PCx], scores[, PCy], xlab=PCx, ylab=PCy,
     pch=c(17,19)[nutrimouse$genotype],
     col=colorRampPalette(c('red','blue'))(nbreaks)[as.numeric(cut(nutrimouse$gene$ALDH3,breaks = nbreal
```


PC2
0.5
0.0
−0.5
−1.0
−1.0
−0.5
0.0
0.5
1.0
1.5
PC1