Principal Component Analysis

UCLouvain - Winter 2023

```
set.seed(1) # for reproducibility of the experiments / random processes

# Libraries
library(tidyverse) # install with install.packages("packagename")
library(broom) # here, useful for "tidying" prcomp objects
library(patchwork) # for displaying several ggplots in a layout
library(GGally) # for pairwise scatter plots
library(plotly) # for interactive visualization
library(ggfortify) # for built-in ggplot2 PCA plots
library(ggrepel) # for avoiding overlapping labels

theme_set(theme_light())
```

Example 1: Taste of most commonly eaten food in the NL

The "Taste, Fat and Texture Database - taste values Dutch Foods" is a database providing the subjective taste of the most commonly eaten food in the NL. It has been compiled by Monica Mars et al., in the context of the "SVT (Smaak, Vet en Textuur)" study. Briefly, trained panelists reported their perceived intensities of the 5 basic tastes, i.e. sweet, salt, sour, bitter and umami, as well as fat sensation for 627 foods. More information regarding the study and the database can be found here.

We load the data `csv` file with

```
tastes <-
  read_csv(
    "data/food_taste_NL/20170202 Sensory database v004.csv",
    show_col_types = FALSE
  )
```

```r
dim(tastes)
```

```
[1] 627  36
```

```r
# str(tastes)
# summary(tastes)
```

We see that the first columns (1 - 12) contain food descriptors, while the remaining columns provide the taste data. Specifically, the taste data contain the number of panelists that tasted the food (`no_`), the mean taste intensity (`m_`), and the standard deviation (`sd_`) or error (`se_`).

The columns we are interested in exploring are those containing the mean taste intensity (i.e., those starting with `m_`)

But we noticed (e.g., with `summary(tastes)` that some food have missing values, so, we remove those food items first.

```r
tastes_complete <-
  tastes %>%
  filter(complete.cases(across(starts_with("m_"))))
nrow(tastes_complete) - nrow(tastes) # number of food items that were removed
```

```
[1] -24
```

Also, to facilitate interpretation down the analysis, we select some food groups we are especially interested in.

```r
tastes_selected <-
  tastes_complete %>%
  filter(Food_group_EN %in%
           c("(non) alcoholic beverages",
             "Bread", "Fruit", "Vegetables",
             "Nuts, seeds and savoury snacks",
             "Pastry, Cakes and Biscuits", "Cheese", "Fish",
            "Meat, meat products and poultry",
             "Milk and milk products"
             )
         )
```

```r
t <- tastes_selected %>% select(starts_with("m_"))
# since we only keep the average value,
# we rename the columns and remove the "m_" prefix
colnames(t) <- colnames(t) %>% str_remove(.,"^m_")
head(t)
```

```
# A tibble: 6 x 6
  sweet  sour bitter umami  salt   fat
  <dbl> <dbl>  <dbl> <dbl> <dbl> <dbl>
1    46    46      3     1     1     5
2    56    20      7     0     2     4
3    51    33      6     0     2     3
4    28    41      8     1     2     8
5     1     1      4     1     1     4
6    10    23      1    33    32    14
```

```r
summary(t)
```

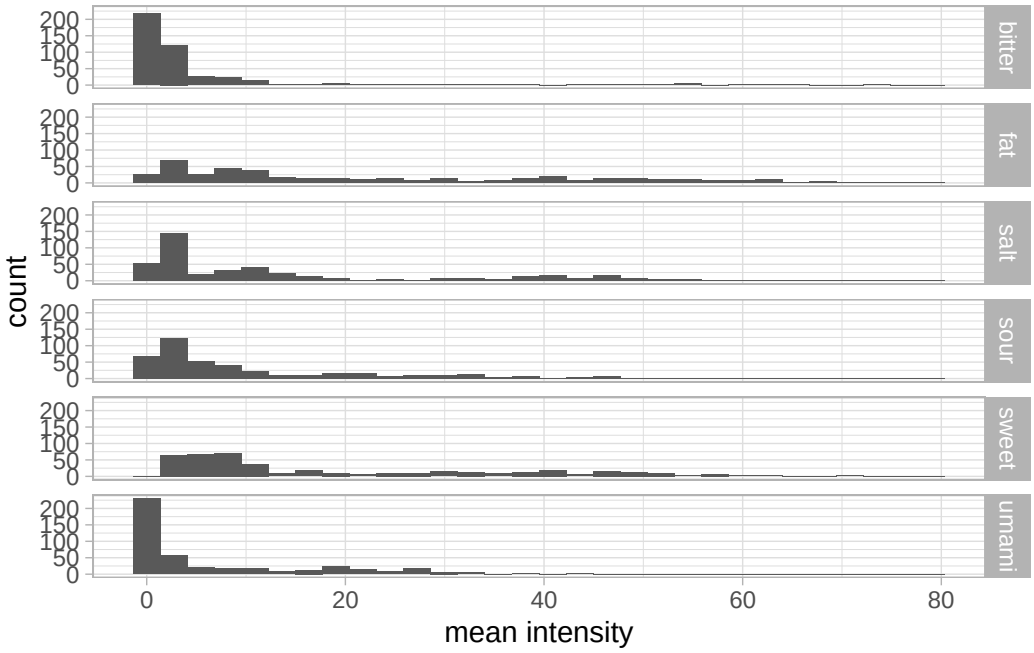
```
     sweet            sour           bitter           umami      
 Min.   : 1.00   Min.   : 0.00   Min.   : 0.000   Min.   : 0.000  
 1st Qu.: 6.00   1st Qu.: 2.00   1st Qu.: 1.000   1st Qu.: 1.000  
 Median :11.00   Median : 6.00   Median : 2.000   Median : 1.000  
 Mean   :19.71   Mean   :12.04   Mean   : 5.673   Mean   : 7.004  
 3rd Qu.:34.00   3rd Qu.:18.75   3rd Qu.: 4.000   3rd Qu.:11.000  
 Max.   :70.00   Max.   :73.00   Max.   :74.000   Max.   :44.000  
      salt             fat       
 Min.   : 0.00   Min.   : 1.00  
 1st Qu.: 2.00   1st Qu.: 6.00  
 Median : 7.00   Median :15.00  
 Mean   :14.47   Mean   :23.66  
 3rd Qu.:18.75   3rd Qu.:40.00  
 Max.   :67.00   Max.   :79.00  
```

Data exploration

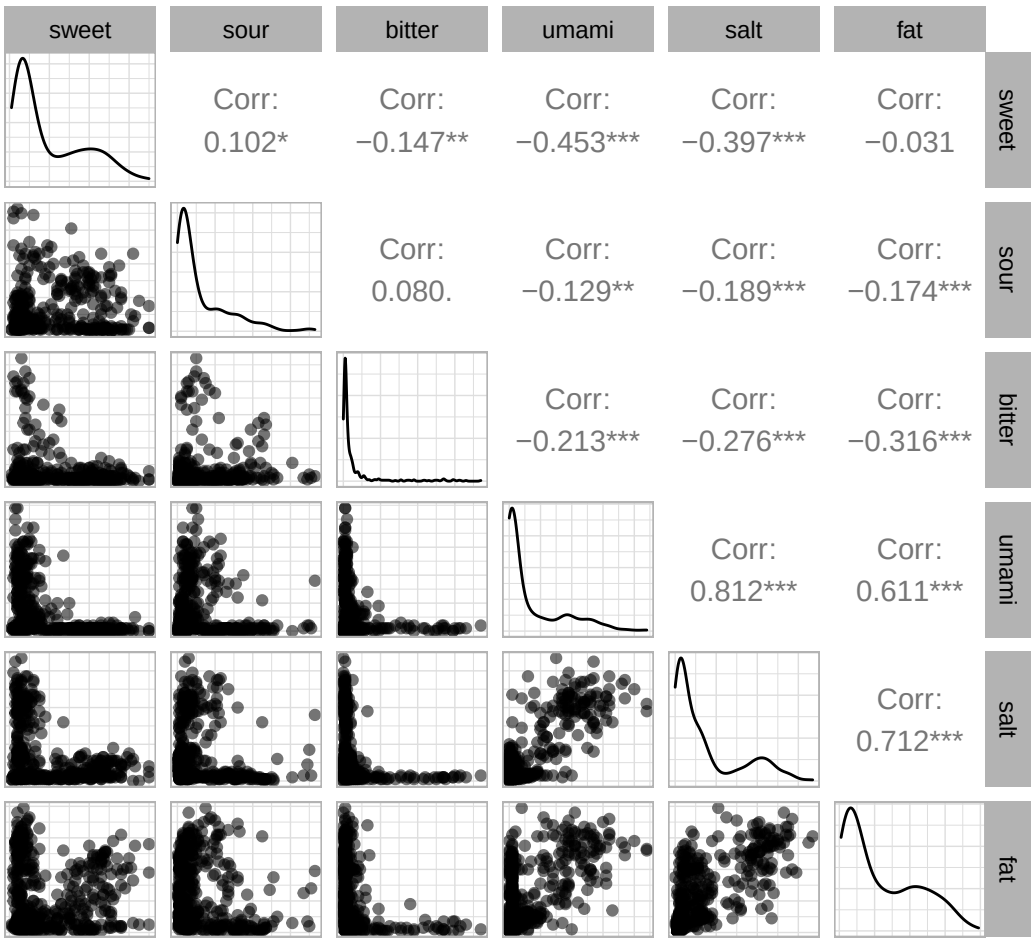
Et first take a quick look at the data and the correlation between variables.

```r
t_long <-
  t %>%
```

```
  mutate(i = row_number()) %>%
  pivot_longer(cols = -i, names_to = "taste", values_to = "mean intensity")

ggplot(t_long, aes(x = `mean intensity`)) +
  geom_histogram(bins = 30) +
  facet_grid(taste ~ .)
```




```
GGally::ggpairs(t, axisLabels = "none", mapping = ggplot2::aes(alpha = 0.25)) +
  theme(strip.text = element_text(color = "black"))
```

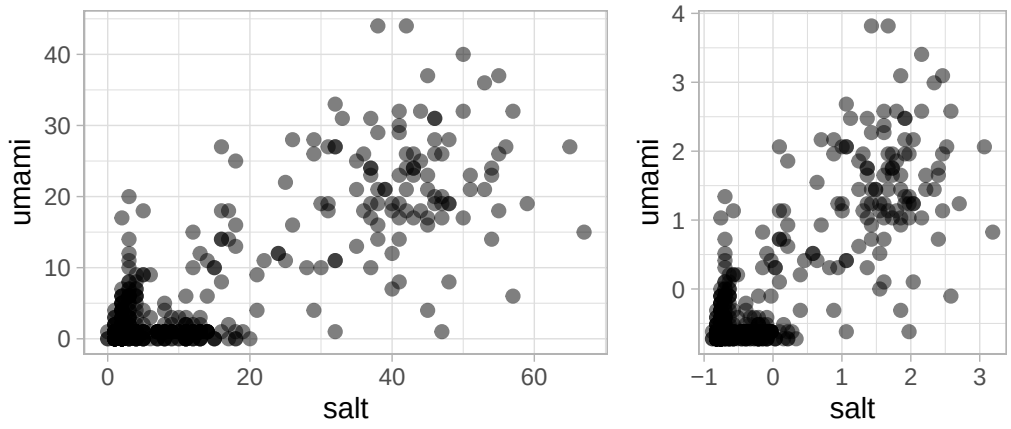


Salt and Umami

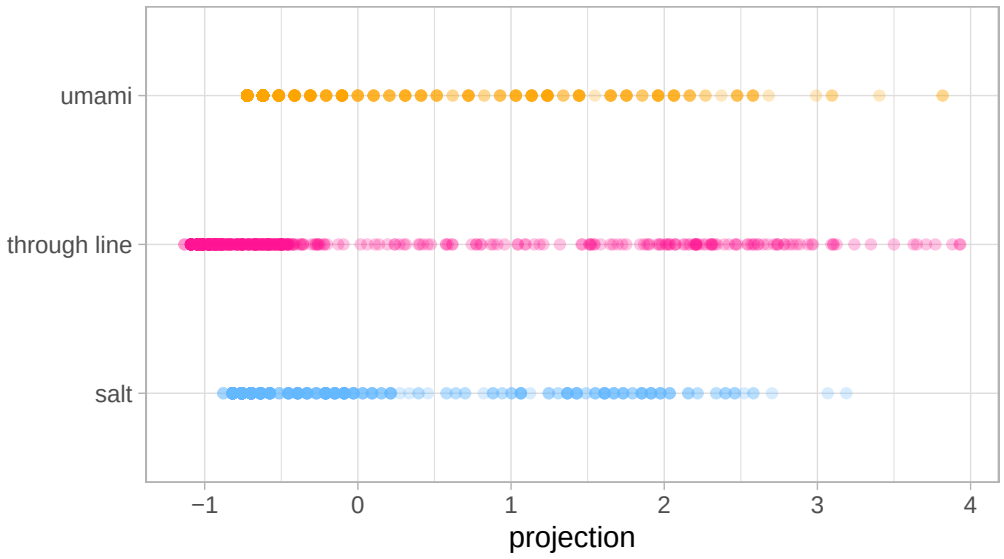
Before performing a PCA on the full dataset with all variables, let's dive in the relationship between the salt and umami flavors and perform a 2D PCA.

```
# scatter plot of the two variables
g_scatter1 <-
  ggplot(t, aes(x = salt, y = umami)) +
  geom_point(size = 2, alpha = 0.5) +
  coord_fixed()

# scatter plot of the standardize variables (subtracting the mean and dividing by the sd)
t_scaled <- t %>% scale() %>% as.data.frame()
g_scatter2 <-
```

```
  ggplot(t_scaled, aes(x = salt, y = umami)) +
  geom_point(size = 2, alpha = 0.5) +
  coord_fixed()

g_scatter1 + g_scatter2
```




```
# finding the direction that maximizes the variance of the projected points
# we'll come back on the use of the `prcomp` function in the next section
pca_t_salt_umami <- prcomp(t_scaled[,c("salt","umami")])

# plotting the projected points onto the 3 axes: the salt, the umami, and the max variance
ggplot(t_scaled) +
  geom_point(aes(x = salt, y = "salt"), col = "steelblue1", alpha = 0.25) +
  geom_point(aes(x = umami, y = "umami"), col = "orange", alpha = 0.25) +
  geom_point(data = pca_t_salt_umami$x %>% as.data.frame(),
             aes(x = PC1, y = "through line"), col = "deeppink", alpha = 0.25) +
  ylab("") + xlab("projection")
```



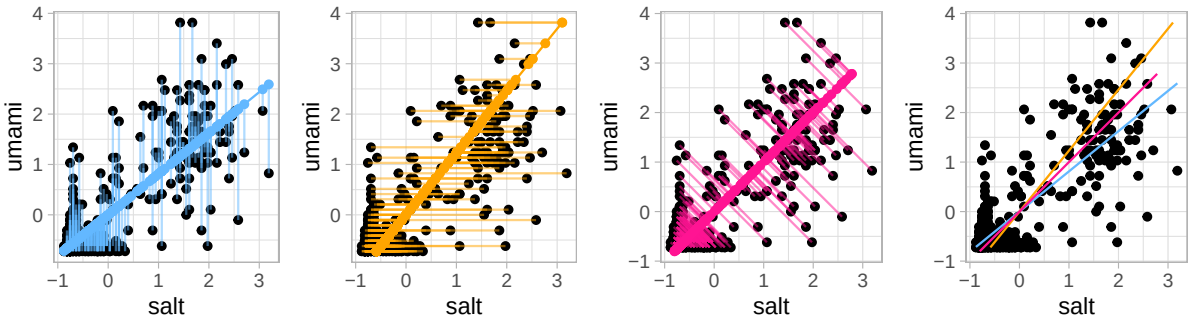

```
pca_t_salt_umami$x[,1] %>% var() # the variance of the projected points on the max varianc
```

```
[1] 1.812316
```

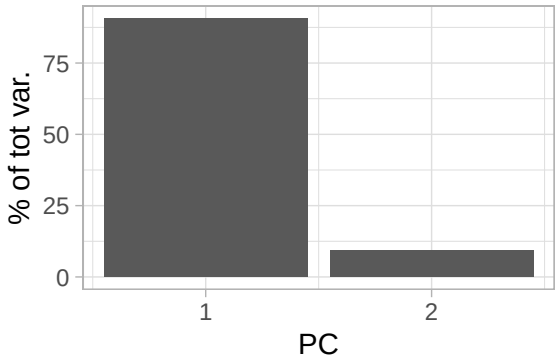
The direction that maximizes the variance is not the same as the directions of the linear models:

```
lm_umami <- lm(umami ~ salt, data = t_scaled)
t_scaled$umami_lm <- lm_umami$fitted.values

lm_salt <- lm(salt ~ umami, data = t_scaled)
t_scaled$salt_lm <- lm_salt$fitted.values


projections_on_PC1 <- pca_t_salt_umami$x
projections_on_PC1[,2] <- 0
projections_on_PC1 <-  projections_on_PC1 %*% t(pca_t_salt_umami$rotation)

t_scaled$salt_pc <- projections_on_PC1[,1]
t_scaled$umami_pc <-  projections_on_PC1[,2]


g_umami <-
  ggplot(t_scaled, aes(x = salt, y = umami)) +
```

```
  geom_point() +
  geom_point(aes(y = umami_lm), col = "steelblue1") +
  geom_line(aes(y = umami_lm), col = "steelblue1") +
  geom_segment(
    aes(xend = salt, yend = umami_lm), col = "steelblue1", alpha = 0.5
    ) +
  coord_fixed()


g_salt <-
  ggplot(t_scaled, aes(x = salt, y = umami)) +
  geom_point() +
  geom_point(aes(x = salt_lm), col = "orange") +
  geom_line(aes(x = salt_lm), col = "orange") +
  geom_segment(
    aes(xend = salt_lm, yend = umami), col = "orange", alpha = 0.5
  ) +
  coord_fixed()  #  + coord_flip()


g_pc <-
  ggplot(t_scaled, aes(x = salt, y = umami)) +
  geom_point() +
  geom_point(aes(x = salt_pc, y = umami_pc), col = "deeppink") +
  geom_line(aes(x = salt_pc, y = umami_pc), col = "deeppink") +
  geom_segment(
    aes(xend = salt_pc, yend = umami_pc), col = "deeppink", alpha = 0.5
  ) +
  coord_fixed()


g_all <-
  ggplot(t_scaled, aes(x = salt, y = umami)) +
  geom_point() +
  geom_line(aes(y = umami_lm), col = "steelblue1") +
  geom_line(aes(x = salt_lm), col = "orange") +
  geom_line(aes(x = salt_pc, y = umami_pc), col = "deeppink") +
  coord_fixed()

(g_umami + g_salt + g_pc + g_all) + plot_layout(ncol = 4)
```




```
tibble(PC = 1:2, sdev = pca_t_salt_umami$sdev) %>%
  mutate(
    var = sdev ^ 2,
    perc = 100 * var/sum(var)
    ) %>%
  ggplot(., aes(x = PC, y = perc)) +
  geom_bar(stat = "identity") +
  ylab("% of tot var.") +
  scale_x_continuous(breaks = c(1:2))
```

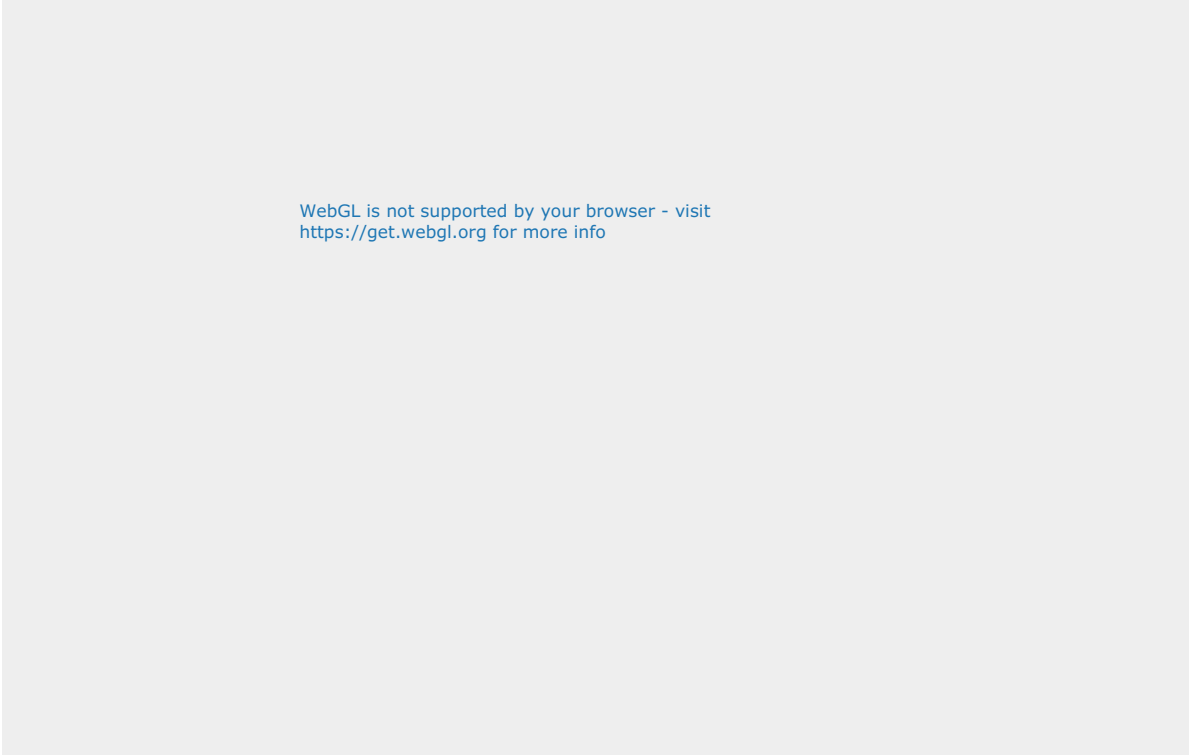


3D toy example

Before performing the PCA on our food dataset, we can explore PCA on a "toy" 3-variable dataset where most of the variance is distributed along one line in the 3D space.

```
set.seed(5) # for the reproducibility of this chunck
N <- 100 # the number of samples
l1 <- rnorm(N) # the latent variable
coeffs <- runif(3, min = -1, max = 1) # the coefficients determining the relationship betw
X <- # the observe variables
```

```r
  l1 %*% t(coeffs) + # Each variable is proportional to the latent variable
  rnorm(3*N, sd = 0.2) # we add some random noise
colnames(X) <- c("x","y","z")

# 3D plot of the data
fig <-
  plotly::plot_ly(
    X %>% as.data.frame(), type = "scatter3d", mode = "markers",
    x = ~x, y = ~y, z = ~z
  )

pca_toy_3d <- prcomp(X, scale = TRUE) # PCA of the toy data

# we compute the projection of the points on the 1st PC line.
projections_on_PC1 <- pca_toy_3d$x
projections_on_PC1[, 2:3] <- 0
projections_on_PC1 <-  projections_on_PC1 %*% t(pca_toy_3d$rotation)
colnames(projections_on_PC1) <- c("x","y","z")

# we add the PC line to our 3D plot
fig <-
  fig %>% plotly::add_lines(
  data = projections_on_PC1 %>% as.data.frame(),
  type = "scatter3d", mode = "line",
  x = ~x, y = ~y, z = ~z
)

fig
```



PCA

To perform a PCA in R, we use the built-in `prcomp` function. It is preferred to the `princomp` function because `prcomp` uses SVD, which is more accurate than using the `eigen` function on the covariance matrix, which is what `princomp` does.

We can also use the `dudi.pca` function from the `ade4` package. This package, along with the `factoextra` package, have a lot of very useful (visualization) functions for PCA. We will come back on this package later. In the meanwhile, coding these functions "from scratch" is a good exercise to understand what is "under the hood".

Scale of the data

While all of our taste variables were measured on a scale from 1 to 100, the range and variance of each variable differ. That is because we filtered for some specific food groups, but also because, inherently, these variables presented differences that are due to the way tastes are perceived by humans.

```
colMeans(t) # we observe substantial differences in means
```

```
    sweet      sour    bitter     umami      salt       fat
19.708520 12.044843  5.672646  7.004484 14.470852 23.663677
```

```r
apply(t, 2, var) # variances
```

```
    sweet      sour    bitter     umami      salt       fat
306.92159 199.33282 139.10608  93.91908 271.31488 425.06866
```

```r
apply(t, 2, range) # and ranges (e.g., umami has a much smaller range)
```

```
     sweet sour bitter umami salt fat
[1,]     1    0      0     0    0   1
[2,]    70   73     74    44   67  79
```

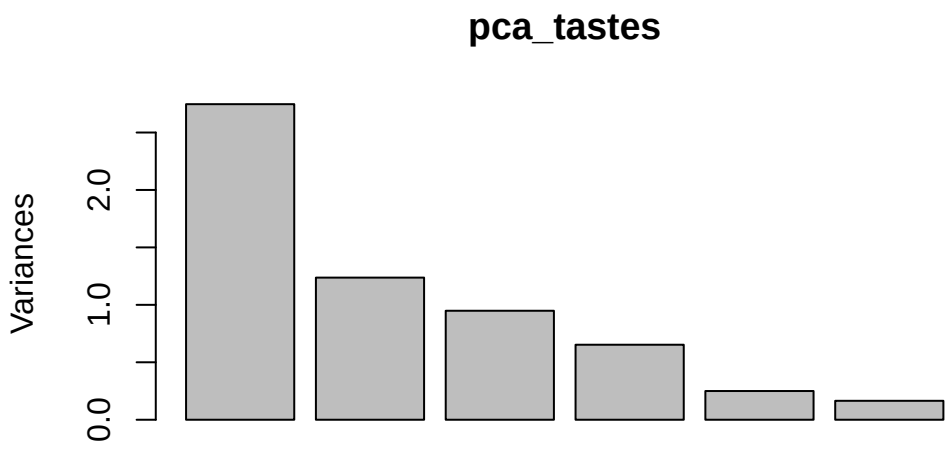
Because of that, we need to scale the data either *before* performing the PCA, or make sure that the option `scale` is `TRUE` in the PCA function itself.

PCA and variance explained by each PC

```r
pca_tastes <- prcomp(t, scale = TRUE) # this returns a `prcomp` object
```

By default, any `prcomp` object comes with a built-in `plot` function, which displays the variance explained by each component.

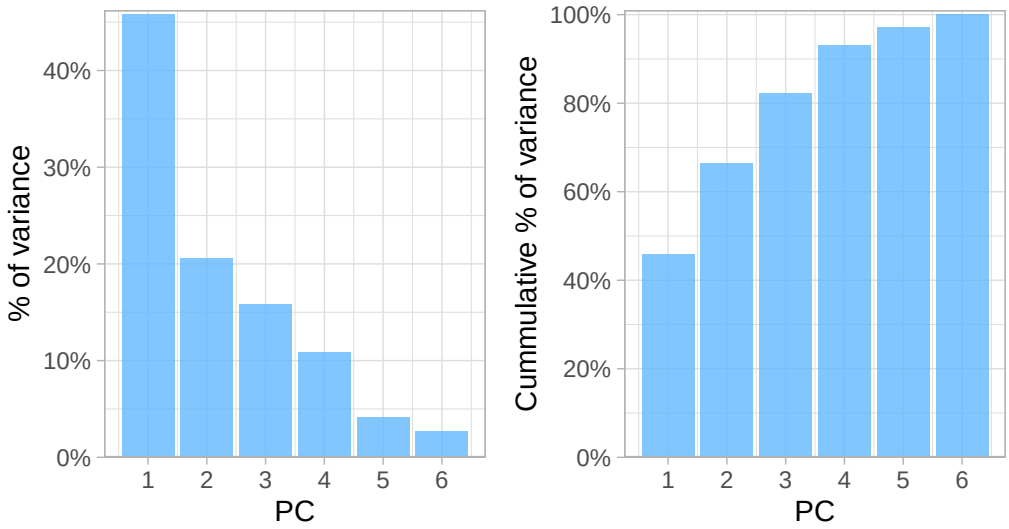
```r
plot(pca_tastes)
```



We can also re-create this visualization using the `ggplot2` package, with some formatting of the PCA results, aided by the `broom` package.

```
pca_var <-
  pca_tastes %>%
  broom::tidy(matrix = "eigenvalues")

plot_pca_var <- function(pca_var) {

  g_var <-
    ggplot(pca_var, aes(PC, percent)) +
    geom_col(fill = "steelblue1", alpha = 0.8) +
    scale_x_continuous(breaks = 1:8) +
    scale_y_continuous(
      "% of variance",
      labels = scales::percent_format(),
      expand = expansion(mult = c(0, 0.01))
    )

  g_cumvar <-
    ggplot(pca_var, aes(PC, cumulative)) +
    geom_col(fill = "steelblue1", alpha = 0.8) +
    scale_x_continuous(breaks = 1:8) +
    scale_y_continuous(
      "Cummulative % of variance",
      breaks = seq(0,1, by = 0.2),
      labels = scales::percent_format(),
      expand = expansion(mult = c(0, 0.01))
    )

  g_var + g_cumvar
}
```

```
plot_pca_var(pca_var)
```



We see that 3 PCs explain over 80% of the variance.

From the original coordinate system to the PC system.

The `prcomp` function returns two other important outputs:

- The `rotation` matrix, which is the matrix that allows to compute the position of the samples in the PC system from the original data
- The `x` matrix, which is the position of the samples in the PC system.

We have that $X = X_0 R$ where X are the sample position in the PC system, X_0 the sample position in the original space, and R the rotation matrix.

```
pca_tastes$rotation
```

```
               PC1         PC2           PC3         PC4         PC5         PC6
sweet  -0.2684148 -0.69540416  0.0002199093 -0.48304468  0.44358387 -0.11944742
sour   -0.1750094  0.01868802 -0.9815845534  0.01295745 -0.06872644 -0.02496032
bitter -0.2278208  0.64187074  0.0398821163 -0.72680576  0.06461954 -0.04568131
umami   0.5416475  0.14434247 -0.1523808153 -0.02213633  0.65865622  0.47775020
salt    0.5646513  0.04008174 -0.0868622194 -0.08733171  0.09134523 -0.80996702
fat     0.4829180 -0.28569996 -0.0643131008 -0.47972543 -0.59343271  0.31421439
```

```
pca_tastes$x %>% as_tibble()
```

```
# A tibble: 446 x 6
      PC1     PC2    PC3      PC4     PC5     PC6
    <dbl>   <dbl>  <dbl>    <dbl>   <dbl>   <dbl>
 1 -2.01  -1.01   -2.15  -0.00965  0.540  -0.147
 2 -1.96  -1.22   -0.311 -0.535    0.908  -0.298
 3 -2.05  -1.04   -1.22  -0.301    0.742  -0.299
 4 -1.66  -0.0669 -1.80   0.0988   0.0553 -0.0382
 5 -0.802  0.787   0.989  1.15    -0.346   0.220
 6  1.93   0.709  -1.25   0.638    1.82    0.337
 7 -2.16   1.78   -0.336 -1.49     0.344  -0.250
 8 -2.03  -0.965  -1.21  -0.358    0.693  -0.280
 9 -1.64   1.11    0.220 -0.716    0.248  -0.0746
10 -2.11   2.46   -2.03  -1.05    -0.0759 -0.0199
# ... with 436 more rows
```

```
all(pca_tastes$x == ((t %>%  scale()) %*% pca_tastes$rotation)) # should be TRUE
```

```
[1] TRUE
```

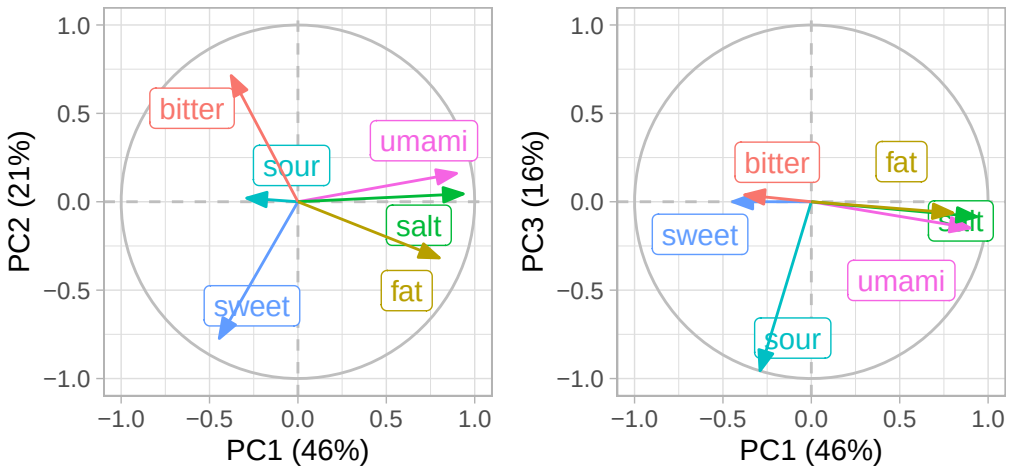
Circle of correlation

Now, we want to understand how the original variables correlate with the new PCs.

To do so, we plot the "circle of correlation", which is a visualization of the correlation between each of the original variable and two selected PCs (usually the first ones as they explain most variation in the data).

```
plot_correlation_circle <- function(data, pca_res, pca_var, PCx = 1, PCy = 2) {

  # first, we compute the correlations between the data in the original axes and the data

  correlations <- cor(data, pca_res$x) %>% as.data.frame()
  correlations$pcx <- correlations[,PCx]
  correlations$pcy <- correlations[,PCy]
  correlations <-
    correlations %>%
    mutate(column = rownames(correlations))

  x_lab <- str_c("PC", PCx, " (",round(100 * pca_var$percent[PCx]),"%)")
  y_lab <- str_c("PC", PCy, " (",round(100 * pca_var$percent[PCy]),"%)")
```

```
  arrow_style <-
    arrow(
      angle = 20, ends = "first", type = "closed", length = grid::unit(8, "pt")
    )

  ggplot(correlations %>% as.data.frame(),
         aes(x = pcx, y = pcy, col = column)) +
    geom_vline(xintercept = 0, col = "gray", linetype = 2) +
    geom_hline(yintercept = 0, col = "gray", linetype = 2) +
    annotate(
      "path",
      x = cos(seq(0, 2*pi,length.out=100)),
      y = sin(seq(0, 2*pi,length.out=100)),
      col = "gray"
    ) +
    ggrepel::geom_label_repel(
      aes(x = pcx, # + 0.05 * pcx / sqrt(pcx^2 + pcy^2),
          y = pcy, # +  0.05 * pcy / sqrt(pcx^2 + pcy^2),
          label = column),
          segment.colour = NA
    ) +
    geom_segment(aes(xend = 0, yend = 0), arrow = arrow_style) +
    xlab(x_lab) +
    ylab(y_lab) +
    guides(col = "none") +
    coord_fixed()

}

g_CC_1_2 <- plot_correlation_circle(data = t, pca_res = pca_tastes, pca_var, 1, 2)

g_CC_1_3 <- plot_correlation_circle(data = t, pca_res = pca_tastes, pca_var, 1, 3)

g_CC_1_2 + g_CC_1_3
```



From these circles of correlations, we make the following observations:

- The *salt* and *umami* flavors are highly with the first principal direction (PC1) mostly discriminate between what is salty or not.
- The *sweet* and *bitter* flavors are most correlated with the second principal direction, but with inverse correlations (*sweet* is anti-correlated with PC2).
- The *sour* flavor has a high correlation with the 3rd PC (but not correlated with the first 2 PC).

The closer to the unitary circle the arrows, the better are these variable represented in the selected PC plane. So, here, the *sour* flavor is not well represented in the PC1-PC2 plane.

We also note that variables that are well represented in a given PC plane and that are highly correlated with each other (e.g., *salt* and *umami* are both well represented in the PC1 - PC2 plane and correlate with each other), have low angles between their correlation circle vectors. That does not hold if variables are not well represented (i.e., have small arrows).

```
cor(t)
```

```
              sweet        sour      bitter      umami       salt         fat
sweet    1.00000000  0.10152612 -0.14694627 -0.4529072 -0.3971764 -0.03096901
sour     0.10152612  1.00000000  0.08014155 -0.1285998 -0.1885879 -0.17400469
bitter  -0.14694627  0.08014155  1.00000000 -0.2125346 -0.2757778 -0.31579780
umami   -0.45290724 -0.12859983 -0.21253457  1.0000000  0.8123162  0.61067023
salt    -0.39717636 -0.18858792 -0.27577777  0.8123162  1.0000000  0.71196754
fat     -0.03096901 -0.17400469 -0.31579780  0.6106702  0.7119675  1.00000000
```

Samples in the PC space

Now that we have a good understanding of how the different variables correlate with the PCs and related with each other, we might be interested in looking at the sample data in the PC coordinate system as it maximizes the variance along the axes.

Instead of the 16 plots showing all the pairwise scatterplots (`GGally::ggpairs`), we hope that one or two plots will suffice in displaying how food relate to each other in terms of tastes.

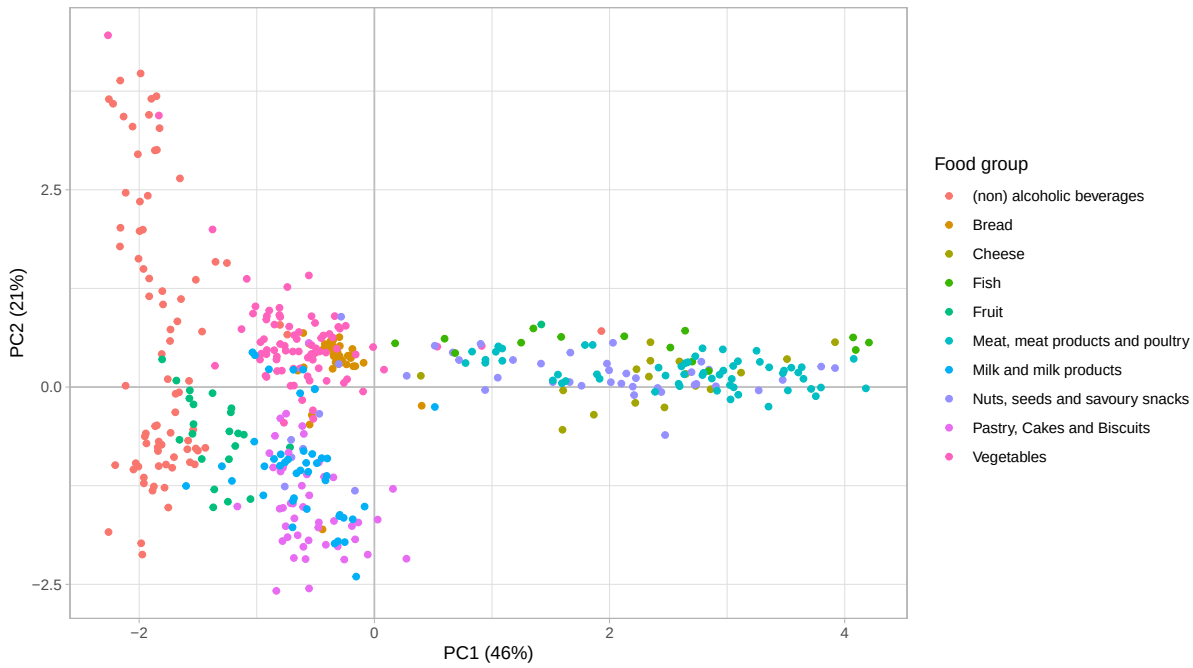
The sample coordinates in this new coordinate system is given by the `x` matrix. Again, we use the functions from the `broom` package to provide objects that are easier to manipulate and (gg)plot than the original `prcomp` object.

```
# Sample PCs + broom::augment add the original dataset to the sample PCs
Sample_PCs <- pca_tastes %>% broom::augment(tastes_selected)

plot_sample_PCs <- function(Sample_PCs, pca_var, PCx, PCy, annot = NULL){

  Sample_PCs$pcx <- Sample_PCs[,str_c(".fittedPC",PCx)] %>% unlist()
  Sample_PCs$pcy <- Sample_PCs[,str_c(".fittedPC",PCy)] %>% unlist()

  g <-
    ggplot(Sample_PCs,
         aes(x = pcx, y = pcy,
             color = Food_group_EN,
             label = Product_description_EN,
             label2 = Food_code)
         ) +
  coord_fixed(pca_var$std.dev[PCy]/pca_var$std.dev[PCx]) +
  geom_vline(xintercept = 0, col = "gray") +
  geom_hline(yintercept = 0, col = "gray") +
  geom_point(size = 1.5) +
  scale_color_discrete("Food group") +
  xlab(str_c("PC", PCx," (",round(100 * pca_var$percent[PCx]),"%)")) +
  ylab(str_c("PC", PCy," (",round(100 * pca_var$percent[PCy]),"%)"))

  if (!is.null(annot)) {
    annot$pcx <- annot[,str_c(".fittedPC",PCx)] %>% unlist()
    annot$pcy <- annot[,str_c(".fittedPC",PCy)] %>% unlist()
    g <-
      g +
      geom_point(data = annot, col = "black", shape = 1, size = 2) +
      geom_text(data = annot,
```

```
                aes(label = Product_description_EN),
                col = "black", vjust = 0, hjust = 0, nudge_x = 0.1
        )
    }

    g

}
```

Let's plot the sample projections in the first 2 PCs and color the samples by the food group they belong to:

```
plot_sample_PCs(Sample_PCs, pca_var, PCx = 1, PCy = 2)
```



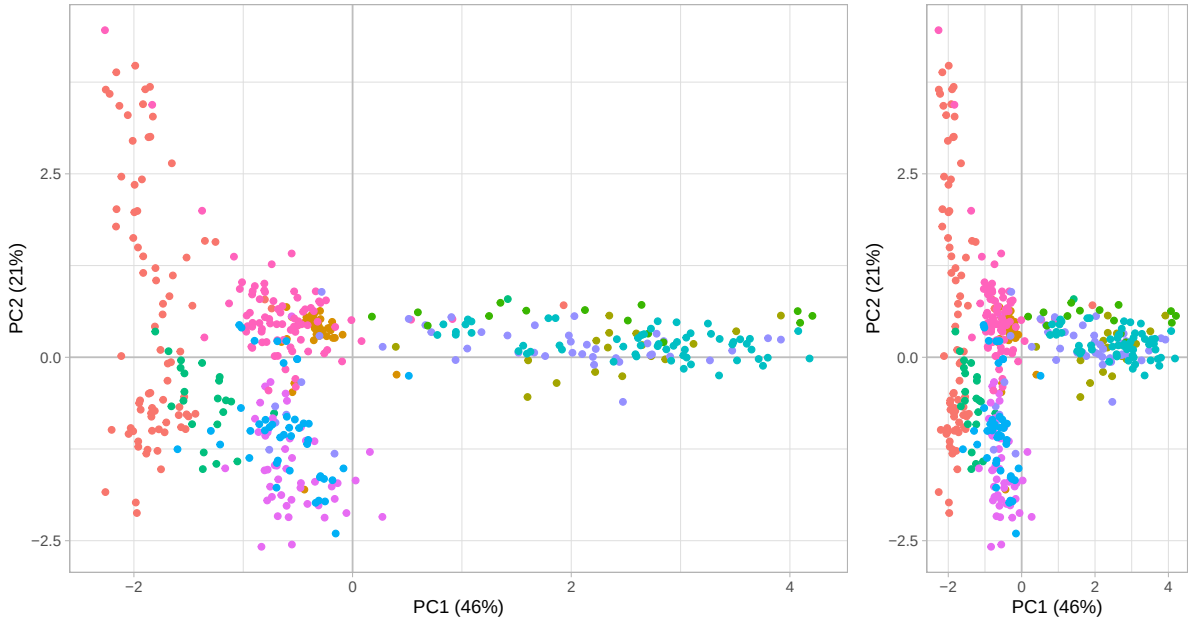
We observe that the food items from the same group tend to cluster together.

For example, most fruits are in the low left corner, in the area dominated by the *sweet* flavor.

One thing to pay attention to is that the scale of the axes is important.

If we compare the two plots below, which of the two plots do you think provides the most accurate representation of the variance along the two axes?

```
(
  plot_sample_PCs(Sample_PCs, pca_var, PCx = 1, PCy = 2) +
    guides(col = "none")
  ) +
  (
    plot_sample_PCs(Sample_PCs, pca_var, PCx = 1, PCy = 2) +
      coord_fixed(ratio = 2) +
      guides(col = "none")
    )
```



The one on the left does. PC1 explains 46% of the variance, so we expect samples to be more spread out along that axis.

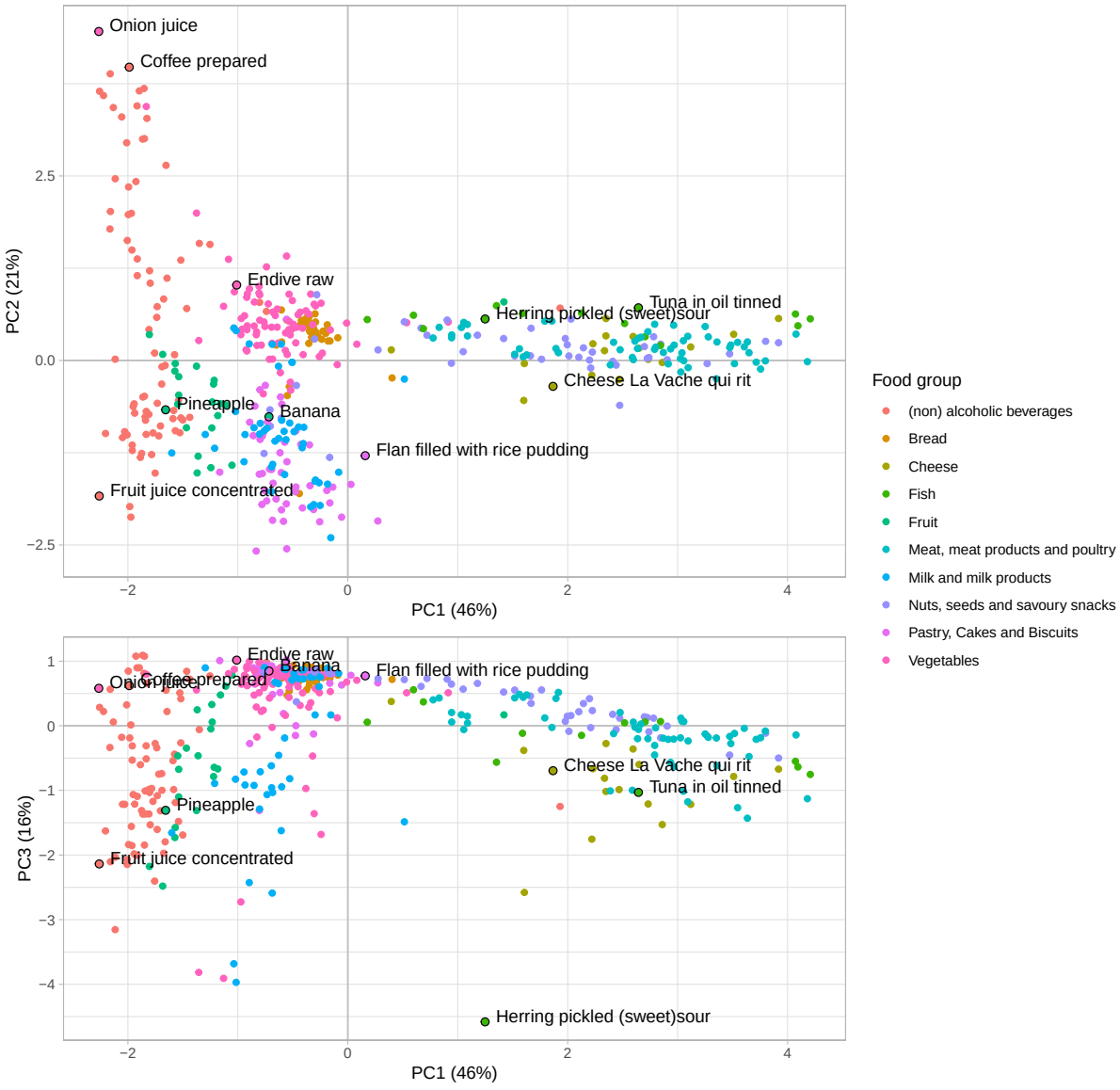
If you go back in the code of the function `plot_sample_PCs`, you will notice that there is a line of code that fixes the coordinate such that the aspect ratio of the plot is proportional to the ratio of the standard deviation explained by each CP.

Remember that to explain at least 80% of the total variation, we need at least 3 CPs.

So, let's visualize the sample projections in each of the 3 first CPs and add annotations for some "landmark" products.

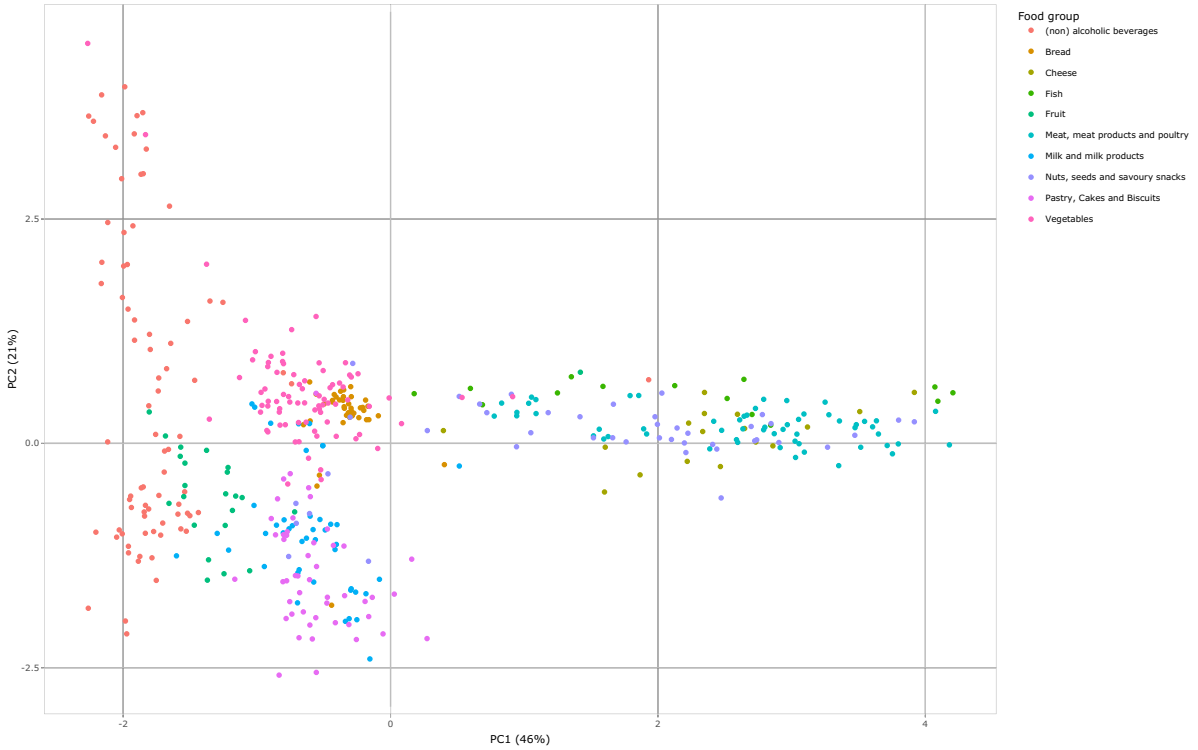
```
selected_food <-
  Sample_PCs %>%
```

```
  filter(Food_code %in%
           #c(395, 1523, 1468, 1885,  2793, 150, 151, 2395, 7, 27272, 2997 )
           c(489, 1655, 632000, 644, 151, 150, 7, 1589, 12121215, 1100)
           )

g_proj_1_2 <- plot_sample_PCs(Sample_PCs, pca_var, 1, 2, annot = selected_food)
g_proj_1_3 <- plot_sample_PCs(Sample_PCs, pca_var, 1, 3, annot = selected_food)

(g_proj_1_2 / g_proj_1_3) + plot_layout(guides = 'collect')
```

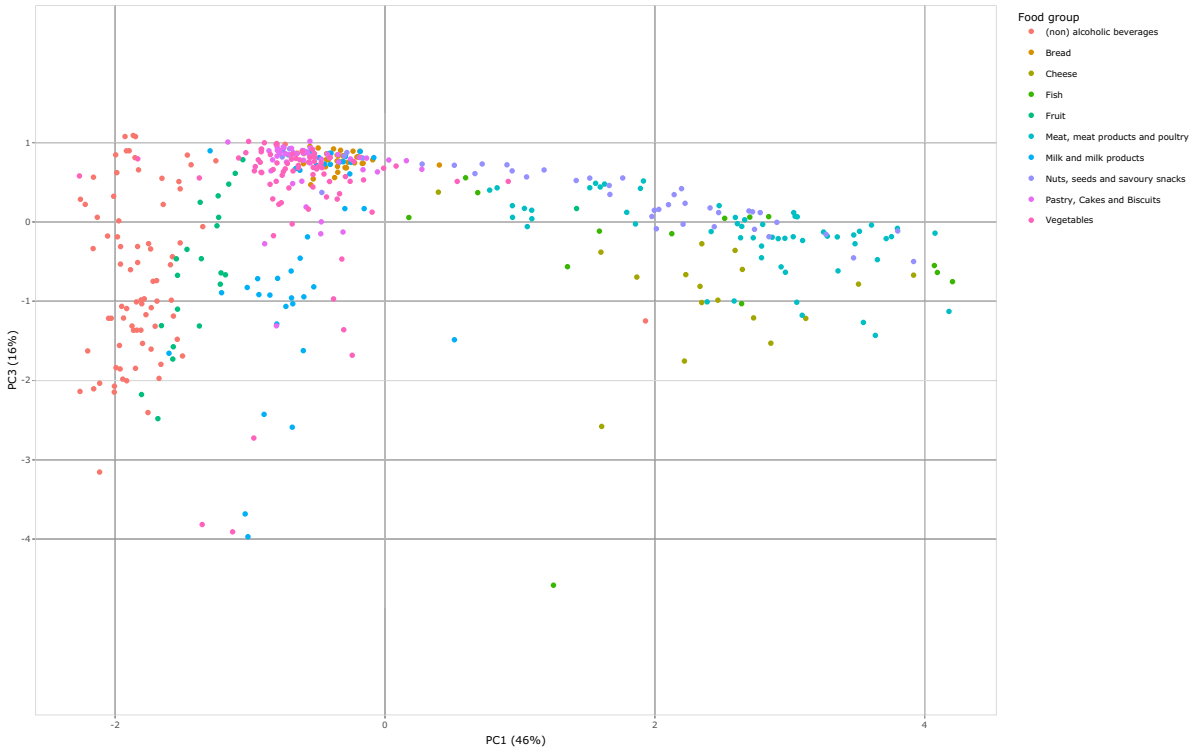


If you are interested in checking more products, interactive visualizations may be useful. You can transform any `ggplot` viz into an interactive one with the `plotly::ggplotly` function. Note that these will not render in pdf format (but they will in html).

```
# interactive view
plot_sample_PCs(Sample_PCs, pca_var, 1, 2) %>% plotly::ggplotly()
```




```
plot_sample_PCs(Sample_PCs, pca_var, 1, 3) %>% plotly::ggplotly()
```



Using the `plotly` library, we can also create 3D visualizations of the first 3 CPs.

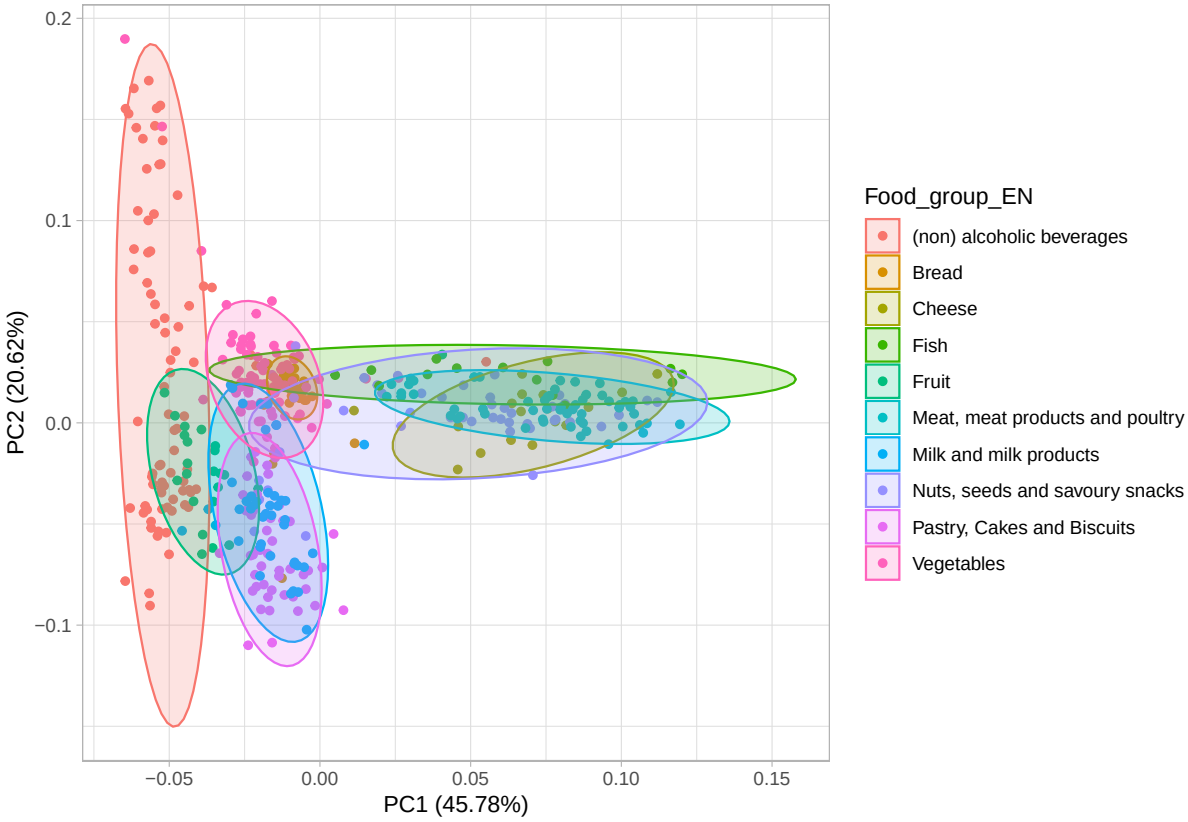
```
# 3D view to explore the main 3 dimensions
PCA_3D <-
  plotly::plot_ly(
    Sample_PCs, type = "scatter3d",
    x = ~.fittedPC1, y = ~.fittedPC2, z = ~.fittedPC3,
    color = ~Food_group_EN,
    size = 0.5
    )
PCA_3D # note that the axes aspect ratio is freely determined here
```

From these visualizations, we observe that most food lie on one of the three first component axis - that might be a consequence of humans limited taste perception: it might be hard for us to distinguish more complex combination or tastes - or we may dislike some combinations (e.g., there might be more food combining sweet and sour than salty and sour or even more complex combinations).

In addition, we observed earlier that food items tended to cluster by food group. We can visualize these clusters by drawing ellipses centered on the center of mass of the food items from each food groups, oriented along the directions of max variations and whose two radii

are proportional to the variation in these directions. We'll come back on these ellipses in later classes.

```
ggplot2::autoplot(
  pca_tastes, data=tastes_selected, colour = "Food_group_EN",
  frame=TRUE, frame.type="t"
  ) +
  coord_fixed(ratio = pca_var$std.dev[2]/pca_var$std.dev[1])
```



Biplots

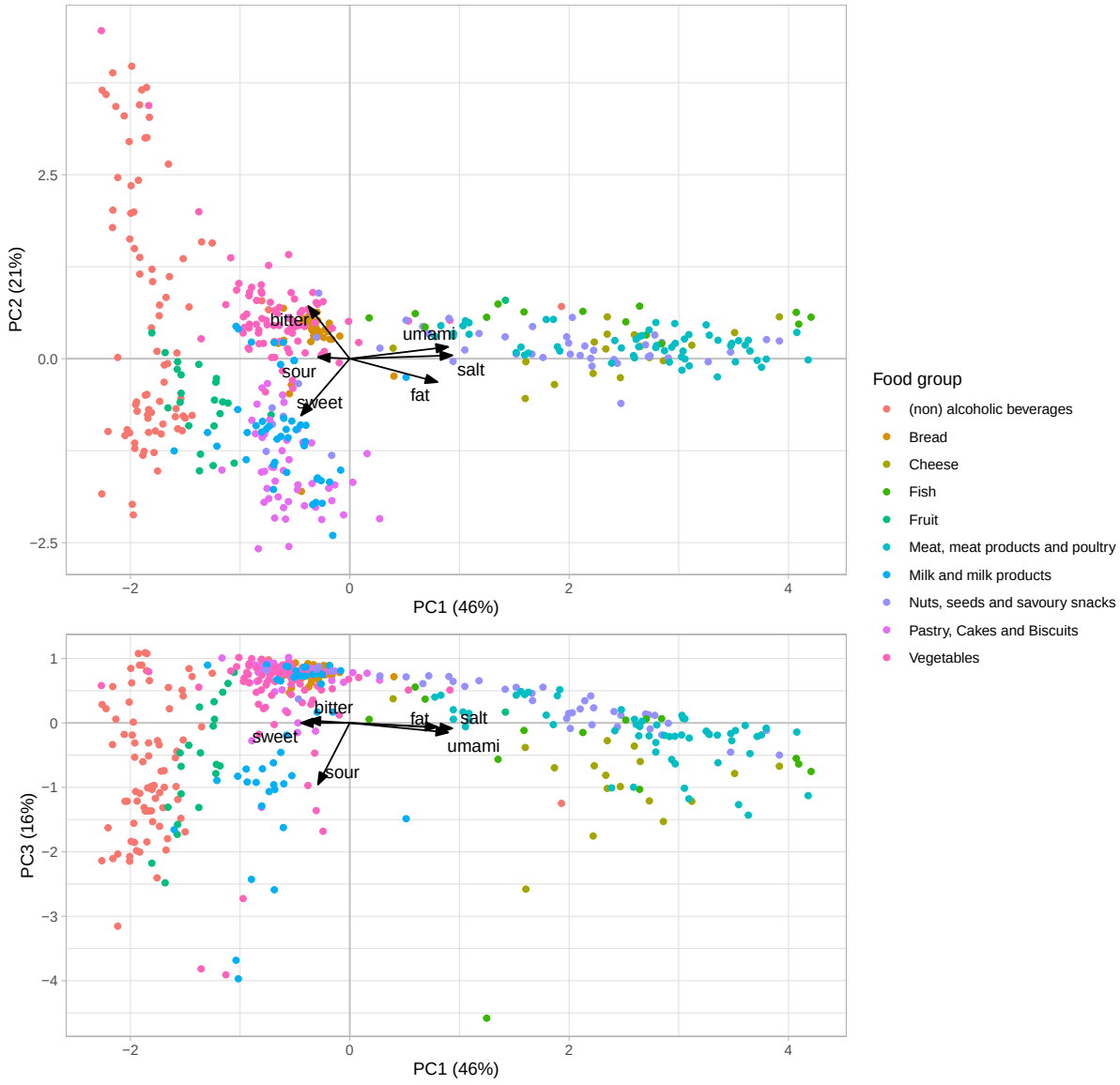
Sometimes, it is useful to display both the sample and the variable projections on the same plot. This is what we call a "biplot".

```
# the default built-in function in R is not the prettiest
# biplot(pca_tastes)
```

```r
# so we can make our own biplot function (based on the two previous ones)
biplot <- function(Sample_PCs, data, pca_res, pca_var, PCx = 1, PCy = 2){

  # sample projections

  Sample_PCs$pcx <- Sample_PCs[,str_c(".fittedPC",PCx)] %>% unlist()
  Sample_PCs$pcy <- Sample_PCs[,str_c(".fittedPC",PCy)] %>% unlist()

  # correlations

  correlations <- cor(data, pca_res$x) %>% as.data.frame()
  correlations$pcx <- correlations[,PCx]
  correlations$pcy <- correlations[,PCy]
  correlations <-
    correlations %>%
    mutate(column = rownames(correlations))

  # axes

  x_lab <- str_c("PC", PCx, " (",round(100 * pca_var$percent[PCx]),"%)")
  y_lab <- str_c("PC", PCy, " (",round(100 * pca_var$percent[PCy]),"%)")

  arrow_style <- arrow(
    angle = 20, ends = "first", type = "closed", length = grid::unit(8, "pt")
  )

  ggplot(Sample_PCs, aes(x = pcx, y = pcy)) +
    geom_vline(xintercept = 0, col = "gray") +
    geom_hline(yintercept = 0, col = "gray") +
    geom_point(aes(color = Food_group_EN), size = 1.5) +
    scale_color_discrete("Food group") +
    geom_text_repel(
      data = correlations,
      aes(x = pcx, # + 0.1 * pcx / sqrt(pcx^2 + pcy^2),
          y = pcy, # +  0.1 * pcy / sqrt(pcx^2 + pcy^2),
          label = column),
          segment.colour = NA
    ) +
    geom_segment(
      data = correlations,
      aes(xend = 0, yend = 0), arrow = arrow_style
```

```
      ) +
    xlab(x_lab) + ylab(y_lab) +
    coord_fixed(pca_var$std.dev[PCy]/pca_var$std.dev[PCx])

}
```

```
biplot_1_2 <- biplot(Sample_PCs, t, pca_tastes, pca_var, PCx = 1, PCy = 2)
biplot_1_3 <- biplot(Sample_PCs,  t, pca_tastes, pca_var, PCx = 1, PCy = 3)
(biplot_1_2 / biplot_1_3) + plot_layout(guides = 'collect')
```



Example 2: random Gaussian data

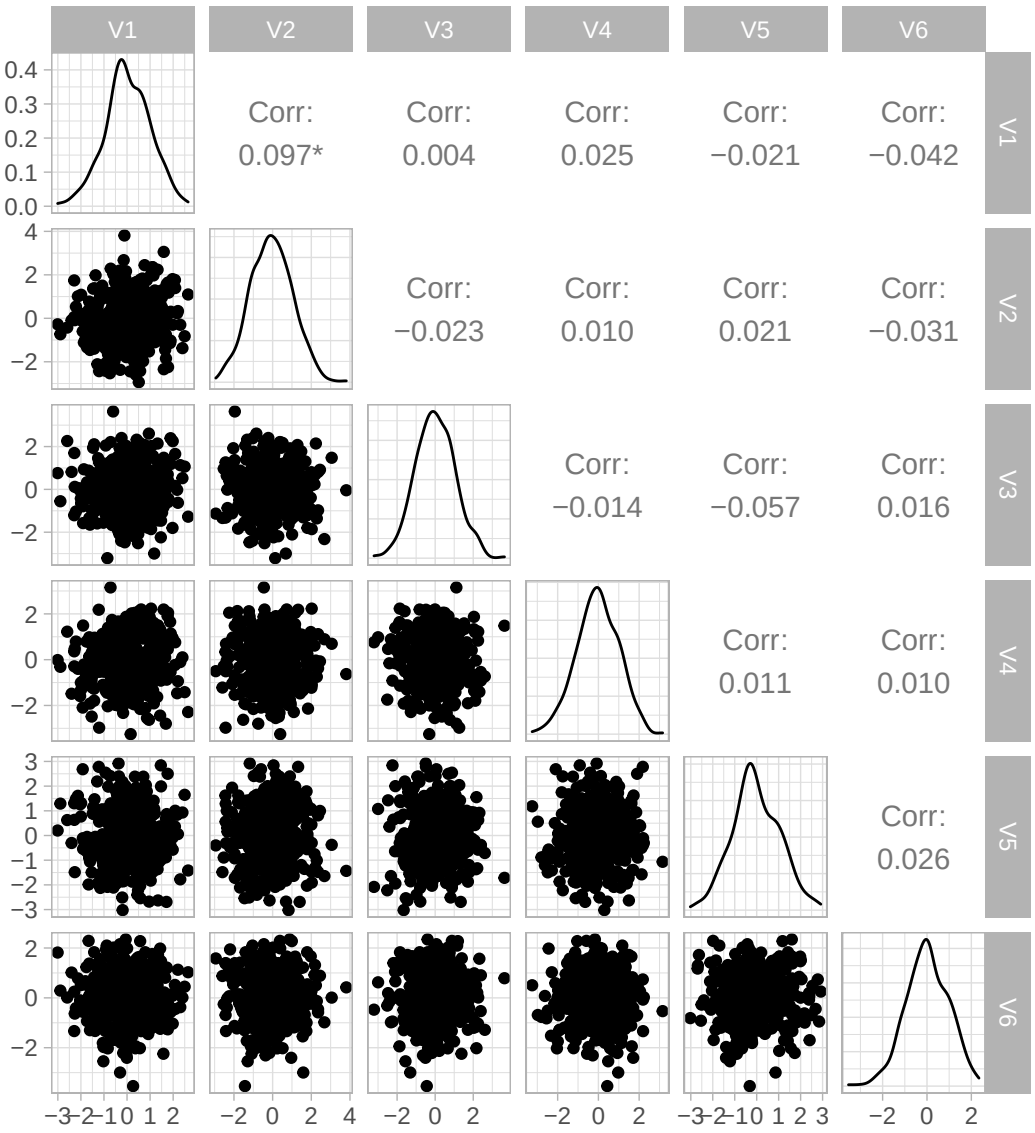
With our first example, we had a 6-variable dataset and we saw that 3 principal components could capture over 80% of the variance. So, it seemed appropriate to conclude that taste perceptions of commonly consumed food in the NL can be describe with these 3 PCs.

Now, not all dataset lie on an underlying lower dimension space. Let's see what happens when we perform a PCA on a 6-dimension dataset composed of **uncorrelated** normally distributed data.

```r
set.seed(1)
sim_data <- matrix(rnorm(prod(dim(t))), nrow = nrow(t), ncol = ncol(t))
```

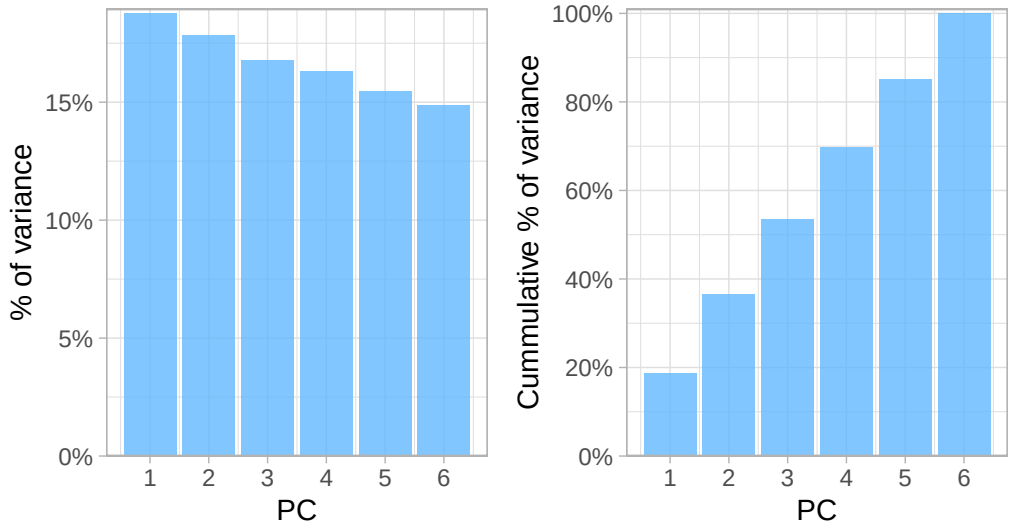
```r
GGally::ggpairs(sim_data %>% as.data.frame(), axisLabels = FALSE)
```

```
Warning in fix_axis_label_choice(axisLabels, c("show", "internal", "none")):
'axisLabels' not in c('show', 'internal', 'none'). Reverting to 'show'
```



```r
pca_sim <- prcomp(sim_data, scale = TRUE) # in theory, we do not need to scale the data as

pca_sim_var <- pca_sim %>% broom::tidy(matrix = "eigenvalues")
```

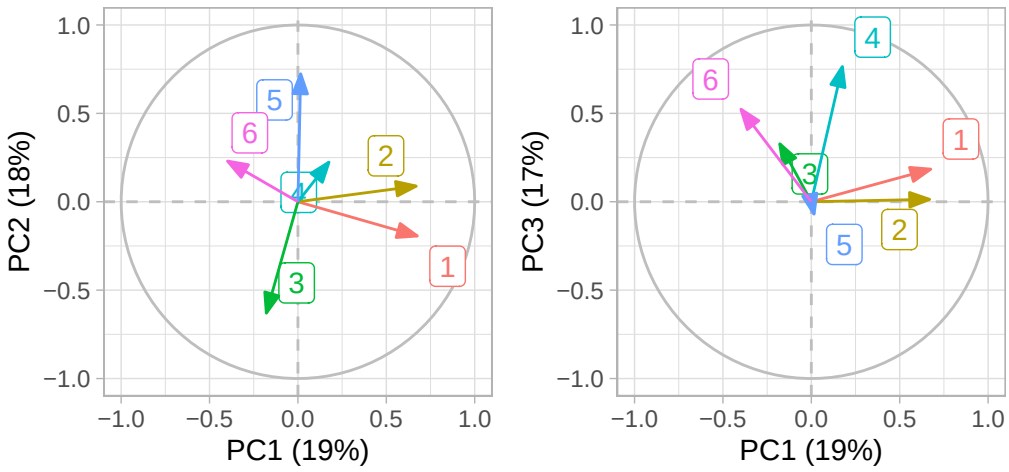
```r
plot_pca_var(pca_sim_var)
```



Now, we see that each variable explains roughly 16% (= 1/6) of the total variance, and that we need 5 out of 6 PC to explain over 80% of the variance.

This indicate that there is likely no linear correlation between the variables and that the data cannot be summarized in a lower dimensional space.

```r
plot_correlation_circle(sim_data, pca_sim, pca_sim_var, 1, 2) +
  plot_correlation_circle(sim_data, pca_sim, pca_sim_var, 1, 3)
```



The correlation circle shows much shorter arrows: most original variables do not correlate very strongly with the principal components

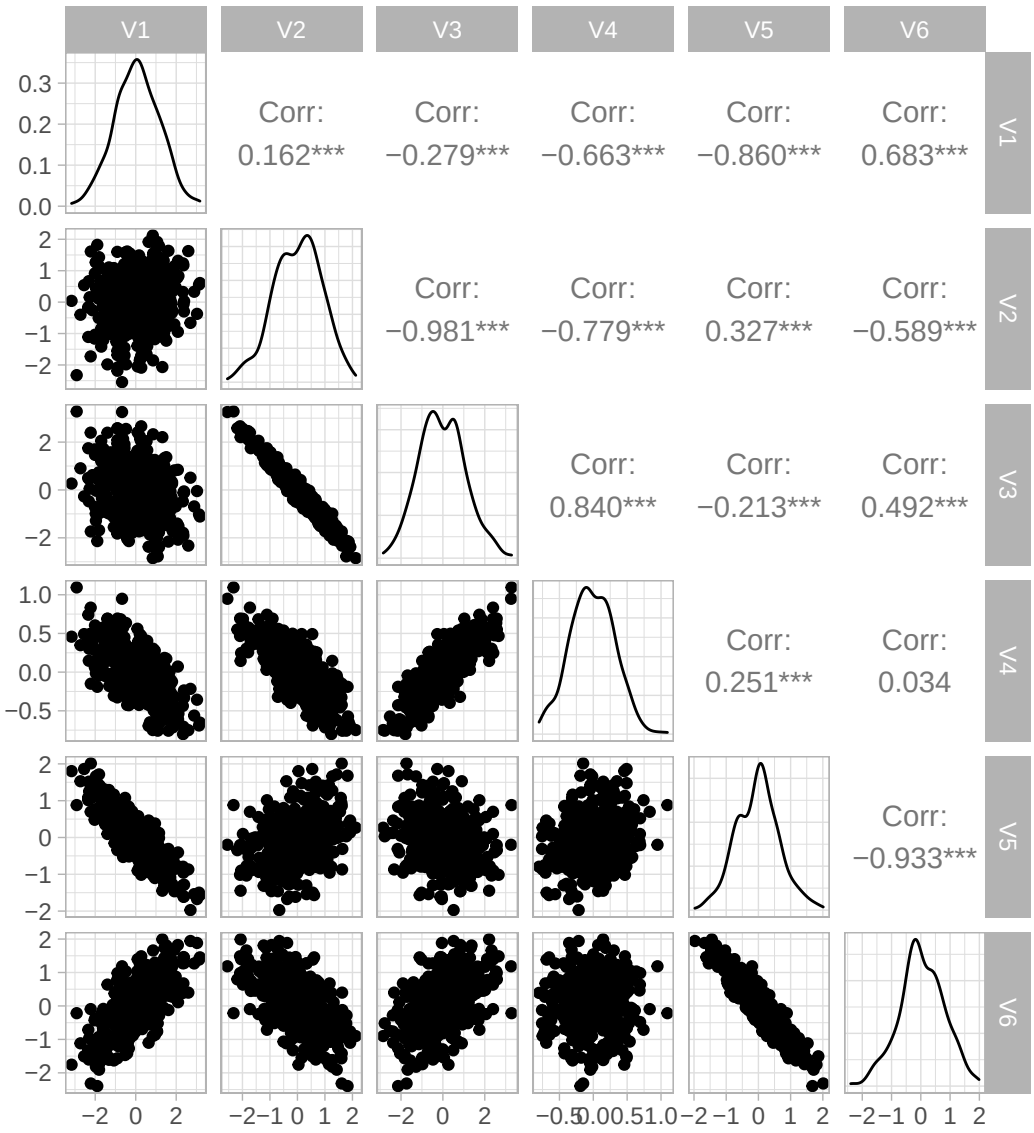
Example 3: Highly correlated variables

Now, let's do the "opposite" exercise and imagine that we have a dataset where the variables are mostly driven by two hidden latent variables. That is, our 6 RVs are *linear combinations* of these two latent variables

```
set.seed(1)
# l1 and l2 are our two latent variables
l1 <- rnorm(nrow(t))
l2 <- rnorm(nrow(t)) # l1 and l2 are independent
coeffs <- matrix(runif(12, -1, 1), 2, 6) # the coefficient of the linear combinations
X <-
  cbind(l1, l2) %*% coeffs +  # linear combination
  rnorm(prod(dim(t)), sd = 0.1) # random noise
```

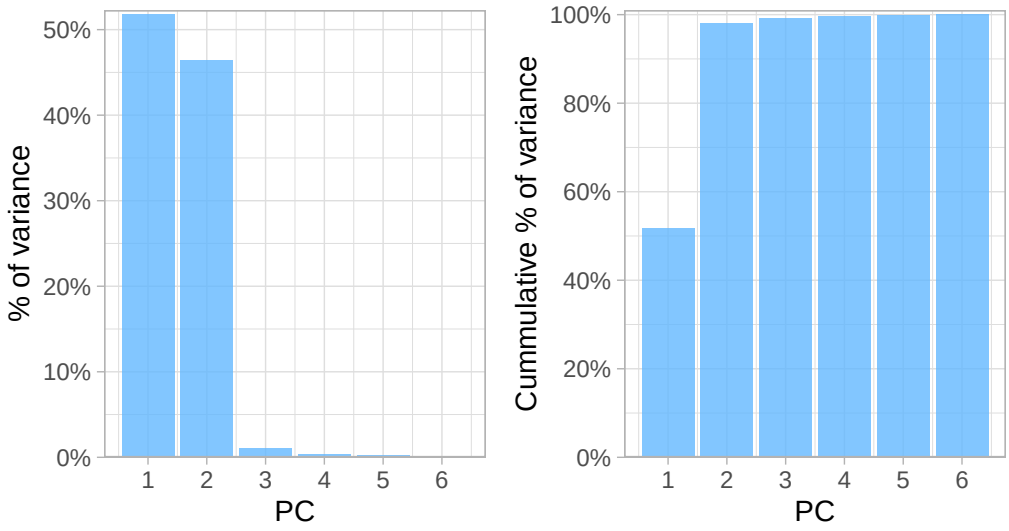
```
GGally::ggpairs(X %>% as.data.frame(), axisLabels = FALSE)
```

```
Warning in fix_axis_label_choice(axisLabels, c("show", "internal", "none")):
'axisLabels' not in c('show', 'internal', 'none'). Reverting to 'show'
```



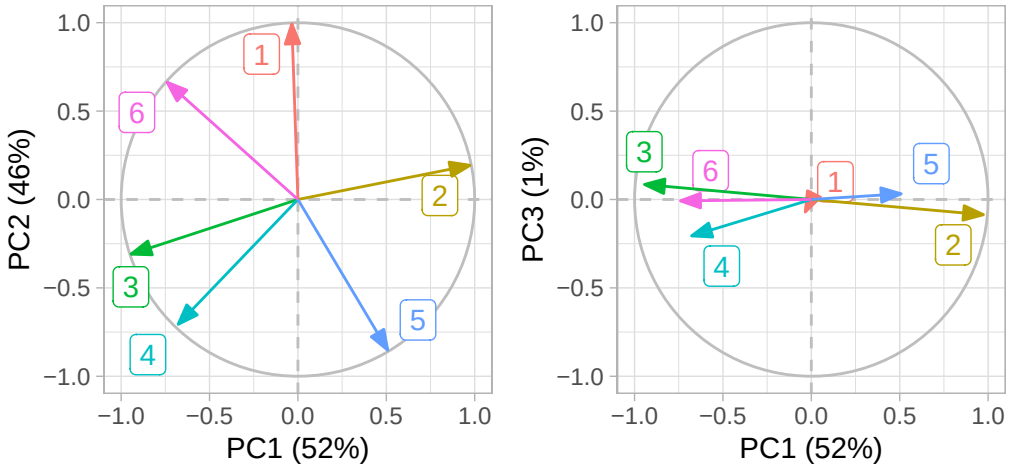

```
pca_sim_2 <- prcomp(X, scale = TRUE)

pca_sim_2_var <- pca_sim_2 %>% broom::tidy(matrix = "eigenvalues")
```

```
plot_pca_var(pca_sim_2_var)
```



We now have a completely different picture: 2 PCs explain almost all of the variance in the data. Since we've simulated the data so that all variables are dependent on the same two latent variable, this should not surprise us.

```
plot_correlation_circle(X, pca_sim_2,  pca_sim_2_var, 1, 2) +
  plot_correlation_circle(X, pca_sim_2,  pca_sim_2_var, 1, 3)
```



We now see that all the arrows are almost of length 1 in the PC1-PC2 plane, which means that all 6 variables are very well represented in the PC1-PC2 space. In contrast, PC3 is not correlated with any of the original variables.

```r
cor(X, pca_sim_2$x)[,1:2]^2 %>% rowSums()
```

```
[1] 0.9872986 0.9852459 0.9864708 0.9575552 0.9850053 0.9877214
```

Circle of correlation vs. *rotations*

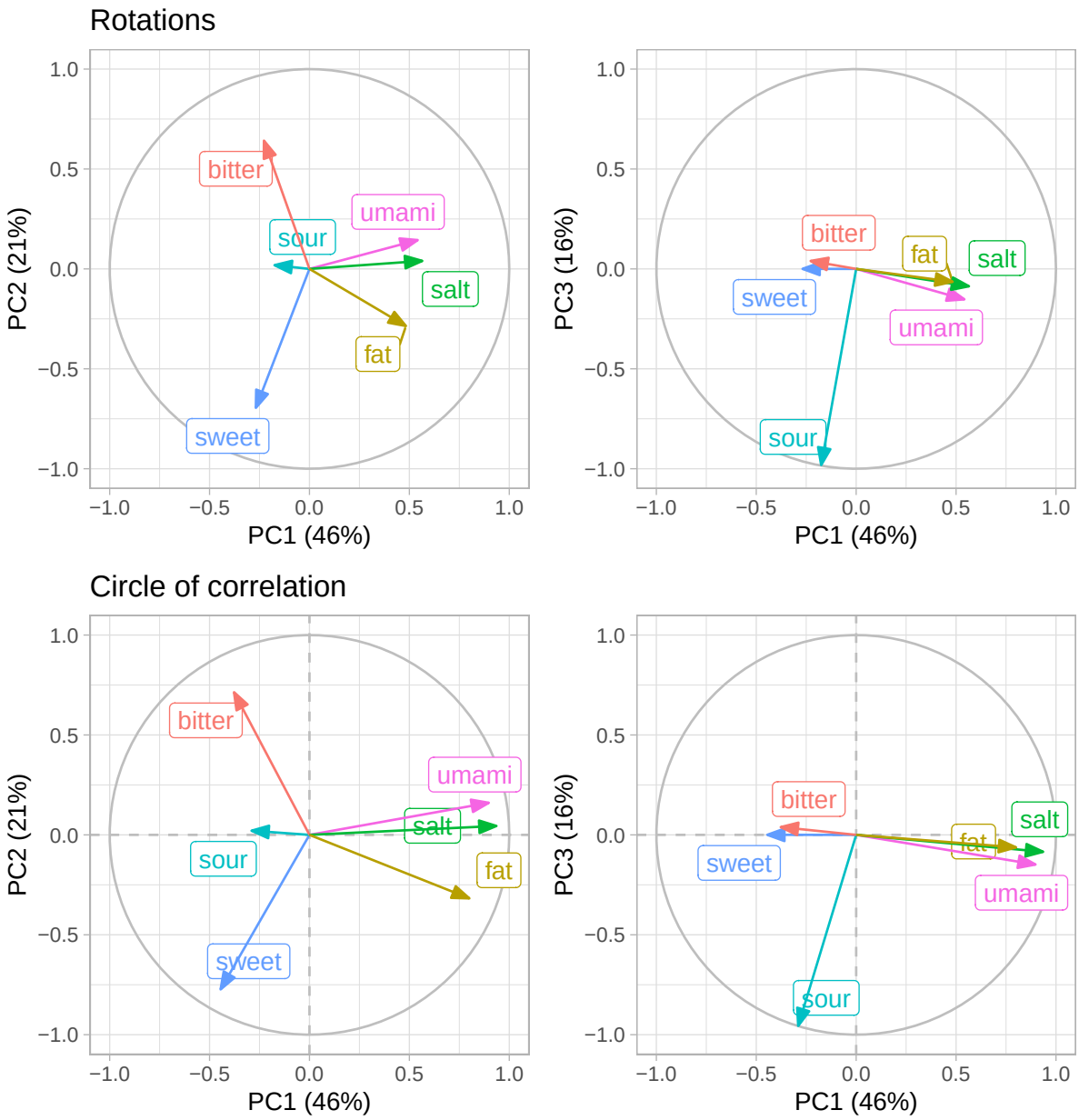
Remember that the `prcomp` function also returns the "rotation" matrix: the matrix that allows to obtain the coordinates of the samples in the PC space from their coordinate in the original dimensions.

We can visualize the projections of this rotation matrix in the first PCs.

```r
# Rotations are in pca_tastes$rotation
rotations_wide <-
  pca_tastes$rotation %>%
  as.data.frame() %>%
  mutate(variable = rownames(pca_tastes$rotation))

plot_rotations <- function(rotations_wide, pca_var, PCx = 1, PCy = 2) {

  arrow_style <-
  arrow(
    angle = 20, ends = "first", type = "closed", length = grid::unit(8, "pt")
  )

  x_lab <- str_c("PC", PCx, " (",round(100 * pca_var$percent[PCx]),"%)")
  y_lab <- str_c("PC", PCy, " (",round(100 * pca_var$percent[PCy]),"%)")

  rotations_wide$pcx <- rotations_wide[, str_c("PC",PCx)] %>% unlist()
  rotations_wide$pcy <- rotations_wide[, str_c("PC",PCy)] %>% unlist()

  ggplot(rotations_wide, aes(x = pcx, y = pcy, col = variable)) +
    annotate(
      "path",
             x = cos(seq(0, 2*pi,length.out=100)),
             y = sin(seq(0, 2*pi,length.out=100)),
      col = "gray"
    ) +
    geom_label_repel(
      aes(x = pcx, # + 0.05 * pcx / sqrt(pcx^2 + pcy^2),
          y = pcy, # +  0.05 * pcy / sqrt(pcx^2 + pcy^2),
```

```
            label = variable)
    ) +
    geom_segment(aes(xend = 0, yend = 0), arrow = arrow_style) +
    xlab(x_lab) +
    ylab(y_lab) +
    guides(col = "none") +
    coord_fixed()

}

g_rot_1_2 <- plot_rotations(rotations_wide, pca_var, PCx = 1, PCy = 2)
g_rot_1_3 <- plot_rotations(rotations_wide, pca_var, PCx = 1, PCy = 3)
```

```
g_rot_1_2 + ggtitle("Rotations") +
  g_rot_1_3 +
  g_CC_1_2 + ggtitle("Circle of correlation") +
  g_CC_1_3
```



Exercises

- In the "Food taste" dataset, how do you interpret that the first 3 PCs are well aligned with 5 of the 6 flavors? What does it say about our taste perception?
- Increase the variance of the random noise in the second simulation (the one with two latent variables). What do you observe?

- Compare the coefficients for the linear combination of the latent variables with the corrleation (circle of correlation), and with the PC1 and PC2 rotations. What do you observe? What makes them different or similar? How could we make the same?
- Explore the `ade4` and `factoextra` packages and the functions
  - `ade4::dudi.pca`,
  - `factoextra::fviz_screeplot` (compare it with our `plot_pca_var`)
  - `factoextra::fviz_pca_var(dudipca_taste)` (compare it with our `plot_correlation_circle`)
  - `factoextra::fviz_pca_ind` (compare it with our `plot_sample_PCs`)