Part 1: Detecting Olive Oil Fraud Using Unsupervised Learning

Derick Malavi

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Introduction

Fraudulent adulteration of **Extra-Virgin Olive Oil (EVOO)** with cheaper oils continues to be a significant concern due to its economic and health implications. Traditional methods for detecting adulteration, such as Gas Chromatography-Mass Spectrometry (GC-MS), are effective but suffer from drawbacks—they are destructive, time-consuming, and costly. As a result, novel non-destructive methods are being explored, including **Near-Infrared Hyperspectral Imaging (NIR-HSI)**.

NIR-HSI is a technique that combines imaging with spectroscopy, capturing both spatial and spectral information across a wide range of wavelengths. This makes it an ideal candidate for detecting subtle changes in EVOO that indicate adulteration. The richness of the spectral data presents a challenge: the data sets are typically large and complex, requiring advanced techniques to reduce dimensionality and reveal underlying patterns. Unsupervised learning methods, such as **Principal Component Analysis (PCA)** and **K-Means clustering**, are crucial tools for addressing this challenge (Malavi et al., 2023).

Principal Component Analysis (PCA)

PCA is a powerful tool for dimensionality reduction, especially in the context of hyperspectral data, where hundreds of spectral bands are captured. By transforming the original variables into a smaller set of uncorrelated principal components, PCA allows us to identify the most significant spectral features contributing to variance in the dataset. This technique is particularly useful in exploring the relationships between different oils and detecting outliers or adulteration patterns without prior labeling of the data.

In this study, PCA was applied to the spectral data obtained from NIR-HSI of pure and adulterated EVOO samples. The goal was to reduce the dimensionality of the data while preserving the most critical information. This not only facilitates visualization but also prepares the data for further unsupervised classification through K-Means clustering.

K-Means Clustering

K-Means clustering is an unsupervised learning technique used to group data points into clusters based on similarity. When applied to the transformed data from PCA, K-Means can group EVOO samples based on their spectral similarities, allowing for the identification of clusters that correspond to pure and adulterated oils. The advantage of K-Means lies in its simplicity and efficiency, making it suitable for large datasets, such as those generated by NIR-HSI.

In this project, K-Means clustering was performed on the principal components derived from the PCA of NIR-HSI data. The clustering process helped to separate the pure EVOO samples from the adulterated ones, providing a preliminary classification without the need for labeled training data. This unsupervised approach serves as a foundational analysis before moving to supervised classification models.

Objectives of Part 1

- **Dimensionality Reduction**: Utilize PCA to reduce the complexity of the hyperspectral data while retaining the most important spectral features for differentiating pure and adulterated EVOO.
- **Unsupervised Classification**: Perform K-Means clustering on the PCA-transformed data to classify EVOO samples based on their spectral characteristics, identifying potential adulteration.
- **Exploratory Data Analysis**: Use PCA and K-Means to uncover hidden patterns in the data, providing insights into how adulteration affects the spectral properties of EVOO.

Dataset

The dataset contains pure samples of extra-virgin olive oil and those adulterated/mixed with different cheaper oils, including safflower, corn, sesame, sunflower, canola, and soybean oils, in concentration ranges of 0-20% (m/m). The samples were analyzed by GC-MS, FTIR, Raman, UV-Vis, and HSI to determine if these methods could identify them as genuine or not.

Load Installed Packages from the R Library for the Analysis

```
warning = FALSE
  suppressWarnings(suppressMessages({
  library(caret)
  library(ggplot2)
  library(dplyr)
  library(readxl)
  library(readr)
  library(janitor)
  library(FactoMineR)
  library(MASS)
  library(factoextra)
  library(rmarkdown)
  library(knitr)
  library(officedown)
  library(quarto)
  library(gtsummary)
  library(pander)
  library(tinytex)
  library(kernlab)}))
```

Load and Inspect Hyperspectral Imaging Data

```
#Load HSI spectra data
hsi<-read_excel("HSI.xlsx")
#Check dimensions
dim(hsi)
```

```
[1] 183 228
```

```
#We have 183 observations and 228 variables
```

```
#Check a few of the column names
colnames(hsi[,c(1:4)])
```

```
[1] "sample_id"    "class_1"      "class_2"      "perc_adulter"
```

```
#Check for any missing values
anyNA(hsi)# There are no missing values
```

```
[1] FALSE
```

```
#Considering that we are conducting a binary classification, we will remove some columns
hsi<-hsi[,-c(1,3)]
table(hsi$class_1)
```

```

Adulterated   Pure EVOO
        144          39
```

```
#convert class_1 to a factor
hsi$class_1<-as.factor(hsi$class_1)
#There are two classes: The oils are either pure/authentic or adulterated
```

```
#Check whether the data is normalized. We want a value between 0 and 1
print(paste('The max value is', max(hsi[,-c(1:4)]),
            'and the min value is', min(hsi[,-c(1:4)])))
```

```
[1] "The max value is 0.827106 and the min value is 0.016328"
```

Load and Inspect Raman Spectroscopy Data

```
#Load Raman spectra data
raman<-read_excel("Raman.xlsx")
#Check dimensions
dim(raman)
```

```
[1]  183 1404
```

```
#We have 183 observations and 1404 variables
```

```
#Bind the data to have the same columns as HSI data
raman<-cbind(hsi[,c(1,2)],raman[,-c(1:3)])
colnames(raman[,c(1:3)])#check whether the changes have been effected
```

```
[1] "class_1"      "perc_adulter" "500"
```

```
table(raman$class_1)#Check the class distribution
```

```
Adulterated   Pure EVOO
        144          39
```

```
class(raman$class_1)#ensure class_1 is a factor
```

```
[1] "factor"
```

```
# Define the normalization function to have values of 0 and 1
min_max_normalize <- function(x) {
  return((x - min(x)) / (max(x) - min(x)))
}
raman<-min_max_normalize(raman[,-c(1:2)])
print(paste('The max value is', max(raman[,-c(1:2)]), 'and the min value is', min(raman[,-c(1:2)]
```

```
[1] "The max value is 1 and the min value is 0"
```

```
anyNA(raman)
```

```
[1] FALSE
```

```
dim(raman)
```

```
[1]  183 1401
```

Load and Inspect FTIR Spectroscopy Data

```
#Load FTIR spectra data
ftir<-read_excel("FTIR.xlsx")
#Check dimensions
dim(ftir)
```

```
[1] 183 919
```

```
#We have 183 observations and 919 variables
```

```
#Bind the data to have the same columns as HSI data
ftir<-cbind(hsi[,c(1,2)],ftir[,-c(1:3)])
colnames(ftir[,c(1:3)])#check whether the changes have been effected
```

```
[1] "class_1"              "perc_adulter"        "470.54590000000002"
```

```
table(ftir$class_1)#Check the class distribution
```

```

Adulterated   Pure EVOO
        144          39
```

```
class(ftir$class_1)#ensure class_1 is a factor
```

```
[1] "factor"
```

```
print(paste('The max value is', max(ftir[,-c(1:2)]),
            'and the min value is', min(ftir[,-c(1:2)])))#The data is OK
```

```
[1] "The max value is 0.6911867 and the min value is 0"
```

```
dim(ftir)
```

```
[1] 183 918
```

Load and Inspect UV-Vis Spectroscopy Data

```r
#Load Uv-Vis spectra data
uv_vis<-read_excel("UVVIS.xlsx")
#Check dimensions
dim(uv_vis)
```

```
[1] 183 125
```

```r
#Bind the data to have the same columns as HSI data
uv_vis<-cbind(hsi[,c(1,2)],uv_vis[,-c(1:4)])
colnames(uv_vis[,c(1:3)])#check whether the changes have been effected
```

```
[1] "class_1"      "perc_adulter" "200"
```

```r
table(uv_vis$class_1)#Check the class distribution
```

```

Adulterated   Pure EVOO
        144          39
```

```r
class(uv_vis$class_1)#ensure class_1 is a factor
```

```
[1] "factor"
```

```r
print(paste('The max value is', max(uv_vis[,-c(1:2)]),
            'and the min value is', min(uv_vis[,-c(1:2)])))#The data is OK
```

```
[1] "The max value is 3.631 and the min value is -0.002"
```

```r
dim(uv_vis)
```

```
[1] 183 123
```

```r
# Define the normalization function to have values of 0 and 1
min_max_normalize <- function(x) {
  return((x - min(x)) / (max(x) - min(x)))
}
uv_vis<-min_max_normalize(uv_vis[,-c(1:2)])
print(paste('The max value is', max(uv_vis[,-c(1:2)]),
            'and the min value is', min(uv_vis[,-c(1:2)])))
```

```
[1] "The max value is 1 and the min value is 0"
```

```r
anyNA(uv_vis)
```

```
[1] FALSE
```

```r
dim(uv_vis)
```

```
[1] 183 121
```

```r
#There are 183 observations and 121 covariates
```

Load and Inspect GC-MS Data

```r
#Load GC-MS data
gc_ms<-read_excel("GC_MS.xlsx")
#Check dimensions
dim(gc_ms)
```

```
[1] 258   9
```

```r
gc_ms$class_1<-factor(gc_ms$class_1)#convert to factor
```

```r
# Define the normalization function to have values of 0 and 1
min_max_normalize <- function(x) {
  return((x - min(x)) / (max(x) - min(x)))
}
gc<-min_max_normalize(gc_ms[,-c(1:2)])
print(paste('The max value is', max(gc), 'and the min value is', min(gc)))
```

```
[1] "The max value is 1 and the min value is 0"
```

```r
anyNA(gc_ms)
```

```
[1] FALSE
```

```r
gc_ms<-cbind(gc_ms[,c(1,2)],gc)
```

Unsupervised Learning

Exploratory Data Analysis by Principal Component Analysis (PCA)

Principal Component Analysis (PCA) is vital for managing the complexity of high-dimensional spectral data from HSI, FTIR, and Raman spectroscopy. It reduces dimensionality, filters noise, extracts key features, improves computational efficiency, and addresses multicollinearity, resulting in more effective and insightful scientific analysis.

Run PCA

```r
hsi_pca<-PCA(hsi[,-c(1,2)],graph = F)#HSI data
hsi_pca$eig[1:10,]#extracting the first 5 components' eigenvalues
```

```
          eigenvalue percentage of variance cumulative percentage of variance
comp 1  178.85959634            79.84803408                          79.84803
comp 2   24.38800697            10.88750311                          90.73554
comp 3   15.63653271             6.98059496                          97.71613
comp 4    1.99152376             0.88907311                          98.60521
comp 5    1.71004670             0.76341371                          99.36862
comp 6    0.44934827             0.20060191                          99.56922
comp 7    0.27623516             0.12331927                          99.69254
comp 8    0.14579543             0.06508724                          99.75763
comp 9    0.11217784             0.05007939                          99.80771
comp 10   0.07117667             0.03177530                          99.83948
```

```r
raman_pca<-PCA(raman[,-c(1,2)],graph = F)#Raman data
raman_pca$eig[1:10,]#extract the first 5 components' eigenvalues
```

```
        eigenvalue percentage of variance cumulative percentage of variance
comp 1  747.843264             53.4555585                          53.45556
comp 2  238.933426             17.0788725                          70.53443
comp 3  149.710682             10.7012639                          81.23569
comp 4   48.348918              3.4559627                          84.69166
comp 5   36.934864              2.6400904                          87.33175
comp 6   26.899571              1.9227713                          89.25452
comp 7   14.313064              1.0230925                          90.27761
comp 8    7.490713              0.5354334                          90.81305
comp 9    6.065781              0.4335798                          91.24662
comp 10   5.423732              0.3876863                          91.63431
```

```r
ftir_pca<-PCA(ftir[,-c(1,2)],graph = F)#FTIR data
ftir_pca$eig[1:10,]#extract the first 5 components' eigenvalues
```

```
         eigenvalue percentage of variance cumulative percentage of variance
comp 1  780.4782964            85.20505419                          85.20505
comp 2  100.1295634            10.93117505                          96.13623
comp 3   21.6371085             2.36212975                          98.49836
comp 4    9.7074370             1.05976386                          99.55812
comp 5    1.6805370             0.18346474                          99.74159
comp 6    0.7223977             0.07886438                          99.82045
comp 7    0.5557826             0.06067496                          99.88113
comp 8    0.4300497             0.04694866                          99.92808
comp 9    0.2056143             0.02244698                          99.95052
comp 10   0.1083039             0.01182357                          99.96235
```

```r
uv_vis_pca<-PCA(uv_vis[,-c(1,2)],graph = F)#UV-Vis data
uv_vis_pca$eig[1:10,]#extract the first 5 components' eigenvalues
```

```
        eigenvalue percentage of variance cumulative percentage of variance
comp 1  88.6460628             74.4924897                          74.49249
comp 2  13.9484433             11.7213809                          86.21387
comp 3   6.6394665              5.5793836                          91.79325
comp 4   4.7728806              4.0108240                          95.80408
comp 5   2.2196215              1.8652281                          97.66931
comp 6   0.8358126              0.7023636                          98.37167
comp 7   0.4465317              0.3752367                          98.74691
comp 8   0.3373078              0.2834519                          99.03036
comp 9   0.2660613              0.2235809                          99.25394
comp 10  0.2102093              0.1766465                          99.43059
```

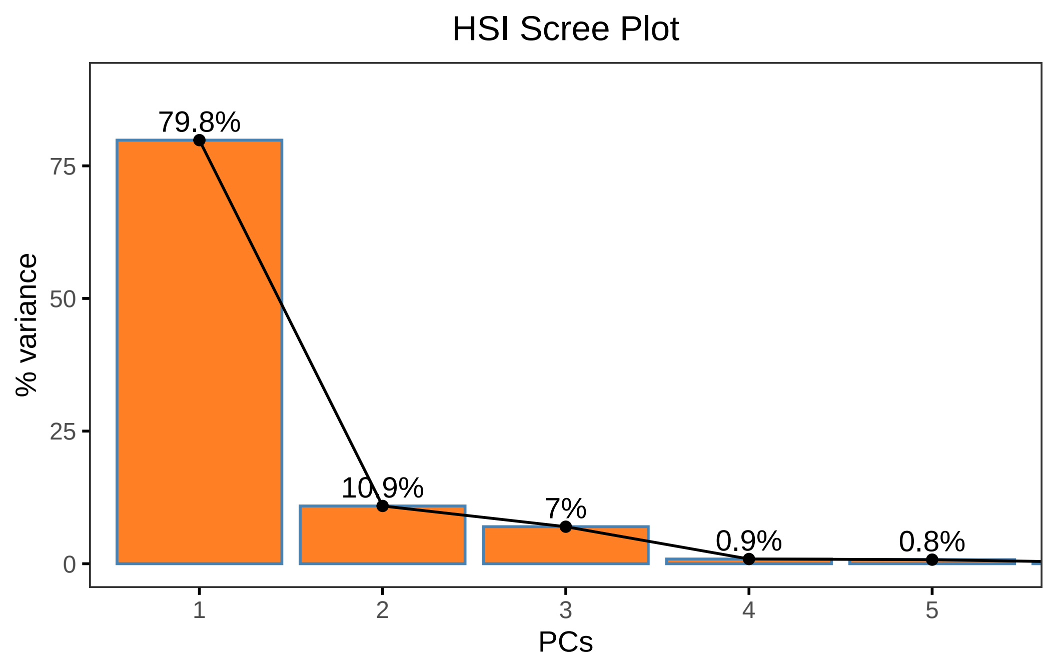
```r
gc_ms_pca<-PCA(gc_ms[,-c(1,2)],graph = F)#GC-MS data
gc_ms_pca$eig[1:7,]
```

```
       eigenvalue percentage of variance cumulative percentage of variance
comp 1  2.7496514             39.2807343                          39.28073
comp 2  1.2952854             18.5040767                          57.78481
comp 3  1.1811070             16.8729572                          74.65777
comp 4  0.8510186             12.1574083                          86.81518
comp 5  0.4893181              6.9902585                          93.80543
comp 6  0.4180069              5.9715265                          99.77696
comp 7  0.0156127              0.2230386                         100.00000
```

Scree Plots

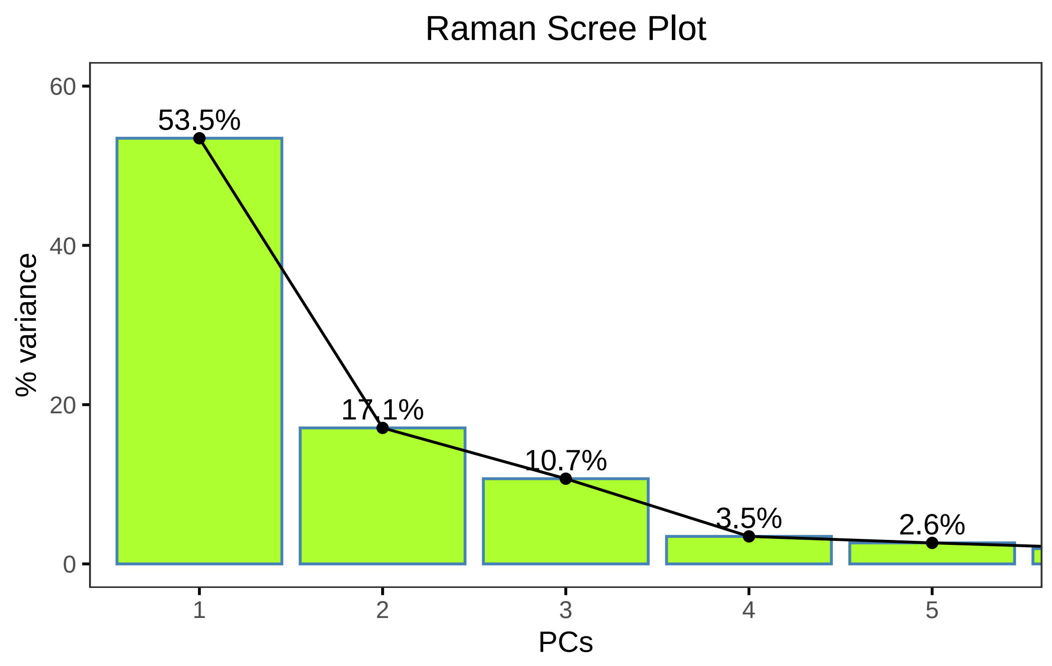
HSI

```r
s1<-fviz_eig(hsi_pca, addlabels = TRUE, ylim = c(0, 90),xlim=c(1,5), main = 'HSI Scree Plot',barf
  theme(plot.title = element_text(hjust = 0.5))+
   theme(panel.grid = element_blank())
print(s1)
```



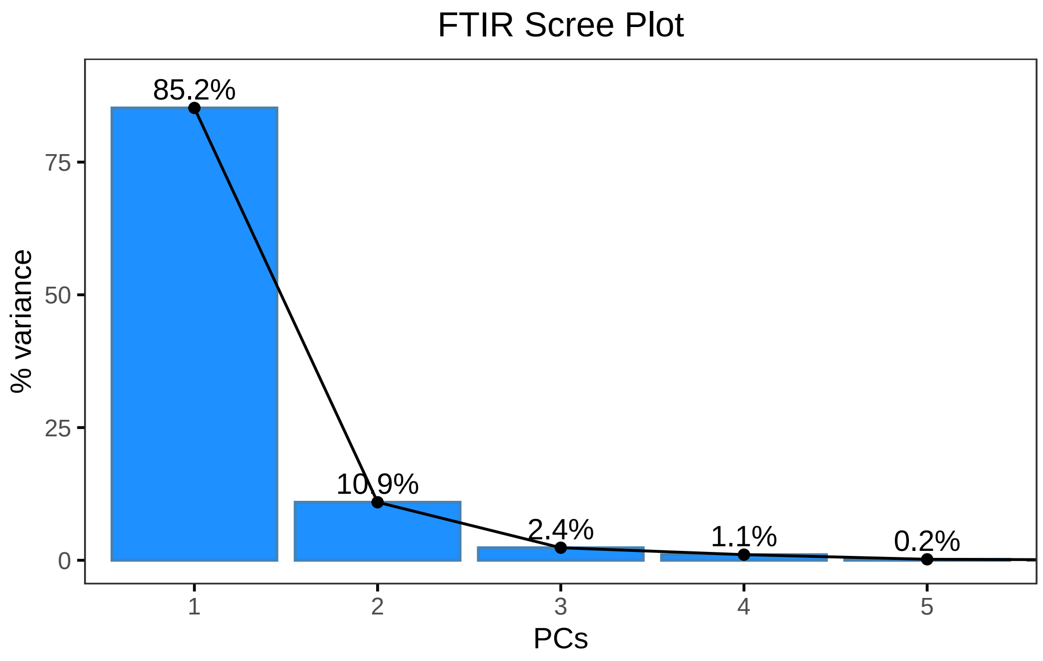
Raman

```
s2<-fviz_eig(raman_pca, addlabels = TRUE, ylim = c(0, 60),xlim=c(1,5),main = 'Raman Scree Plot',b
  theme(plot.title = element_text(hjust = 0.5))+
   theme(panel.grid = element_blank())
print(s2)
```



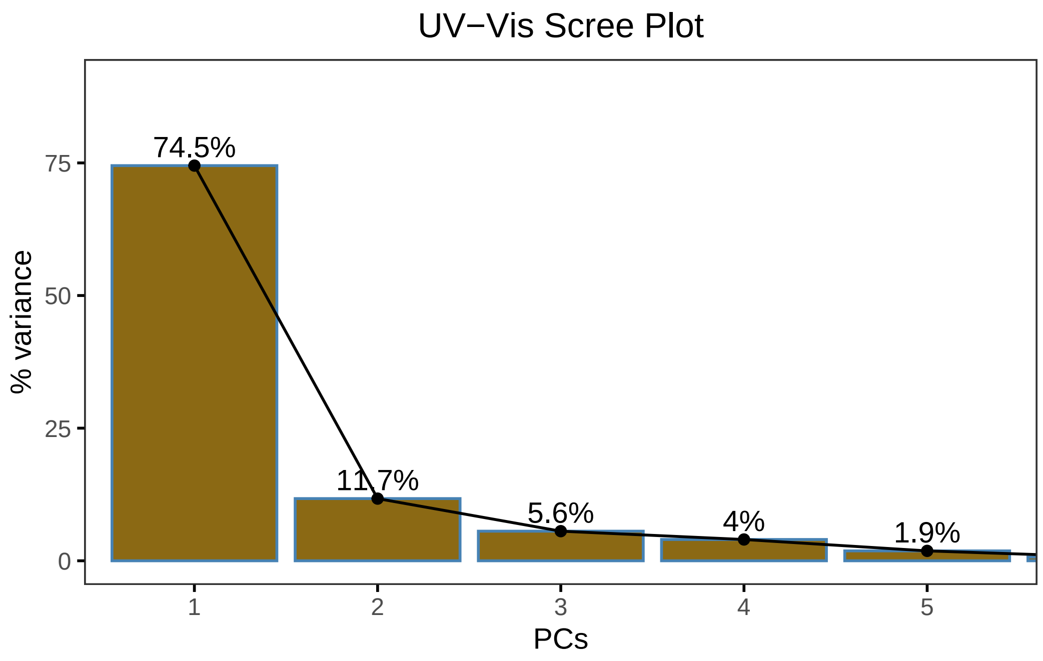
FTIR

```
s3<-fviz_eig(ftir_pca, addlabels = TRUE, ylim = c(0, 90),xlim=c(1,5),main = 'FTIR Scree Plot',bar
  theme(plot.title = element_text(hjust = 0.5))+
    theme(panel.grid = element_blank())
print(s3)
```

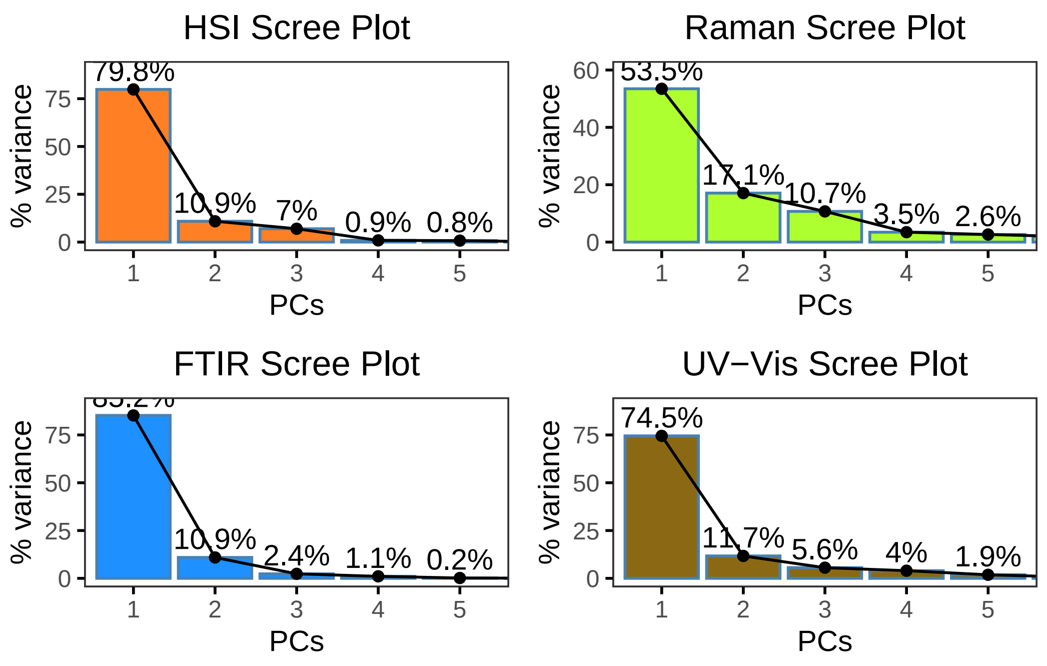


Uv-Vis

```
s4<-fviz_eig(uv_vis_pca, addlabels = TRUE, ylim = c(0, 90),xlim=c(1,5),main = 'UV-Vis Scree Plot'
  theme(plot.title = element_text(hjust = 0.5))+
  theme(panel.grid = element_blank())
print(s4)
```

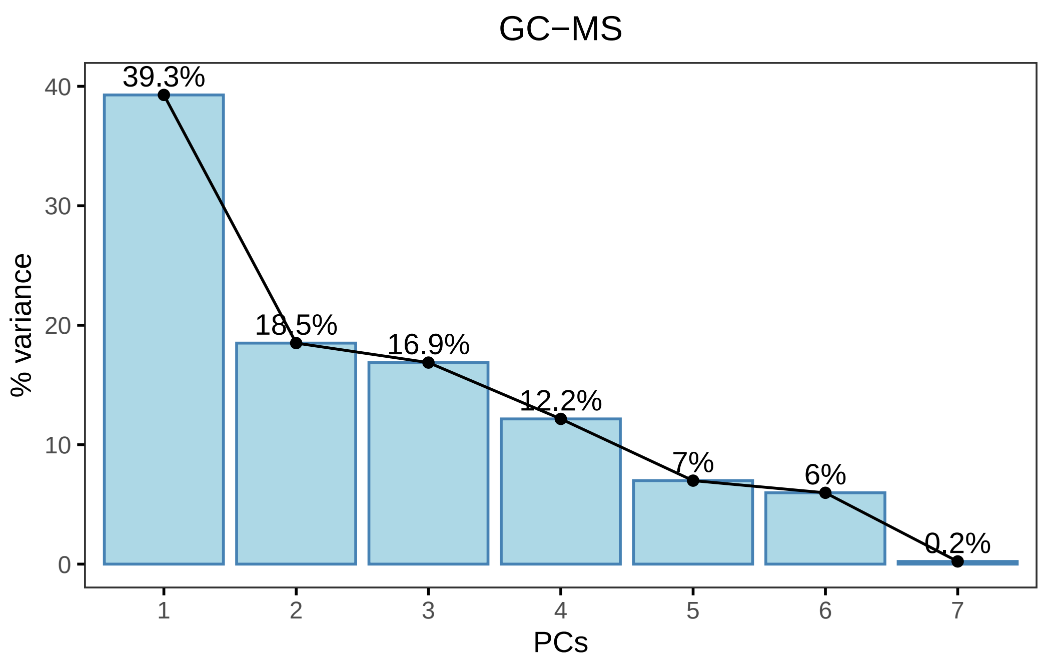


```
#Patch together the scree plots
gridExtra::grid.arrange(s1,s2,s3,s4, nrow =2)
```



GC-MS

```
s5<-fviz_eig(gc_ms_pca, addlabels = TRUE, ylim = c(0, 40),main = 'GC-MS',barfill = "lightblue",hj
  theme(plot.title = element_text(hjust = 0.5))+
   theme(panel.grid = element_blank())

print(s5)
```



- As observed from the data, **more than 80% of the variation** in the data from each of the spectroscopic technique can be explained by the the first 3 PCs.

Visualization of PC Scores

Different principal components will be examined to visualize any patterns from our data. The next step will be to create a new data frame for each technique to be used in subsequent analysis.

```
#HSI Data
hsi_new<-as.data.frame(hsi_pca$ind$coord) #Extract the PCs
colnames(hsi_new)<-c("PC_1","PC_2", "PC_3","PC_4","PC_5")
hsi_new<-cbind(hsi[,c(1,2)],hsi_new)#Bind with the dependent variables
head(hsi_new)
```

```
#Raman Data
raman_new<-as.data.frame(raman_pca$ind$coord) #Extract the PCs
colnames(raman_new)<-c("PC_1","PC_2", "PC_3","PC_4","PC_5")
raman_new<-cbind(hsi[,c(1,2)],raman_new)#Bind with the dependent variables
head(raman_new)
```

```
#FTIR Data
ftir_new<-as.data.frame(ftir_pca$ind$coord) #Extract the PCs
colnames(ftir_new)<-c("PC_1","PC_2", "PC_3","PC_4","PC_5")
ftir_new<-cbind(hsi[,c(1,2)],ftir_new)#Bind with the dependent variables
head(ftir_new)
```

```
#Uv_Vis Data
uvvis_new<-as.data.frame(uv_vis_pca$ind$coord) #Extract the PCs
colnames(uvvis_new)<-c("PC_1","PC_2", "PC_3","PC_4","PC_5")
uvvis_new<-cbind(hsi[,c(1,2)],uvvis_new)#Bind with the dependent variables
head(uvvis_new)
```

```
#GC-MS Data
gc_new<-as.data.frame(gc_ms_pca$ind$coord) #Extract the PCs
colnames(gc_new)<-c("PC_1","PC_2", "PC_3","PC_4","PC_5")
gc_new<-cbind(gc_ms[,c(1,2)],gc_new)#Bind with the dependent variables
head(gc_new)
```

PC Plots

```
# HSI PC Plot
p1 <- hsi_new %>%
  ggplot(mapping = aes(x = PC_1, y = PC_2, shape = class_1, color = perc_adulter)) +
  geom_point() +
  labs(x = "PC1 (79.8%)", y = "PC2 (10.9%)",title = "HSI PC Plot", shape = "Oil type", color = "P
  theme_bw() +
  theme(
    panel.border = element_rect(color = 'black', fill = NA),
    panel.grid = element_blank(),
    axis.text.x = element_text(color = 'black', size = 10),
    axis.text.y = element_text(color = 'black', size = 10),
    aspect.ratio = 1,
    axis.title.x = element_text(size = 9),
    axis.title.y = element_text(size = 9),
    plot.title = element_text(size = 9, hjust = 0.5),
    legend.title = element_text(size = 8),
    legend.text = element_text(size = 6),
     legend.position = "none") +
  scale_color_gradient(low = "#000000", high = "red") +
  stat_ellipse(aes(group = class_1),
               level = 0.95,
               geom = "polygon", alpha = 0.2,
               color = 'black', linewidth = 0.6)
```

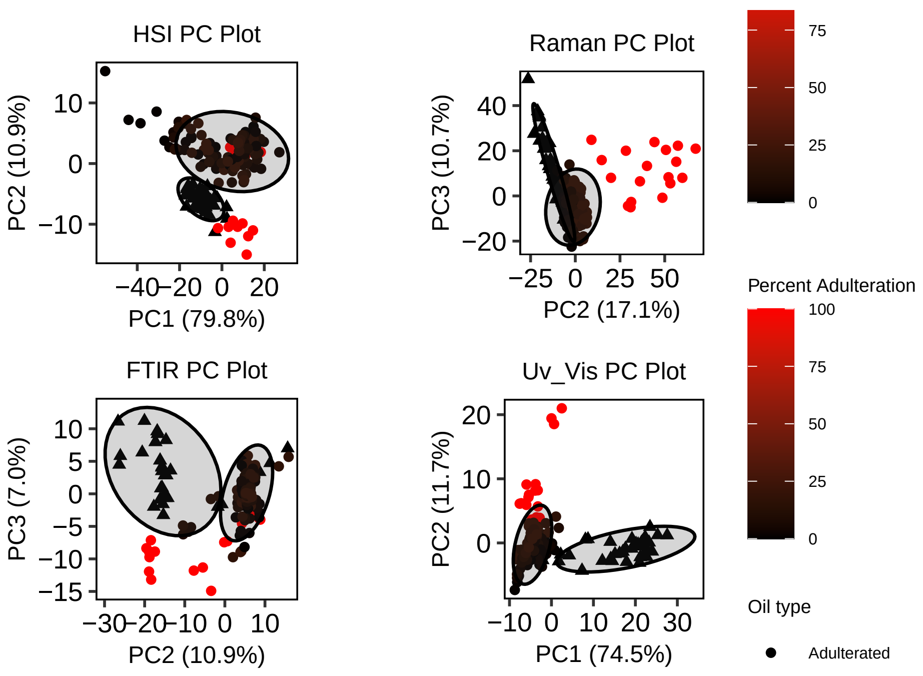
```
#Raman Plot
p2 <- raman_new %>%
  ggplot(mapping = aes(x = PC_2, y = PC_3, shape = class_1, color = perc_adulter)) +
  geom_point() +
  labs(x = "PC2 (17.1%)", y = "PC3 (10.7%)",title = "Raman PC Plot", shape = "Oil type", color =
  theme_bw() +
  theme(
    panel.border = element_rect(color = 'black', fill = NA),
    axis.text.x = element_text(color = 'black', size = 10),
    panel.grid = element_blank(),
    axis.text.y = element_text(color = 'black', size = 10),
    aspect.ratio = 1,
    axis.title.x = element_text(size = 9),
    axis.title.y = element_text(size = 9),
    plot.title = element_text(size = 9, hjust = 0.5),
    legend.title = element_text(size = 7),
    legend.text = element_text(size = 6)) +
  scale_color_gradient(low = "#000000", high = "red") +
  stat_ellipse(aes(group = class_1),
               level = 0.95,
               geom = "polygon", alpha = 0.2,
               color = 'black', linewidth = 0.6)
```

```
#FTIR Plot
p3 <- ftir_new %>%
  ggplot(mapping = aes(x = PC_2, y = PC_3, shape = class_1, color = perc_adulter)) +
  geom_point() +
  labs(x = "PC2 (10.9%)", y = "PC3 (7.0%)",title = "FTIR PC Plot", shape = "Oil type", color = "P
  theme_bw() +
  theme(
    panel.border = element_rect(color = 'black', fill = NA),
    axis.text.x = element_text(color = 'black', size = 10),
    panel.grid = element_blank(),
    axis.text.y = element_text(color = 'black', size = 10),
    aspect.ratio = 1,
    axis.title.x = element_text(size = 9),
    axis.title.y = element_text(size = 9),
    plot.title = element_text(size = 9, hjust = 0.5),
    legend.title = element_text(size = 7),
    legend.text = element_text(size = 6),
     legend.position = "none") +
  scale_color_gradient(low = "#000000", high = "red") +
  stat_ellipse(aes(group = class_1),
               level = 0.95,
               geom = "polygon", alpha = 0.2,
               color = 'black', linewidth = 0.6)
```

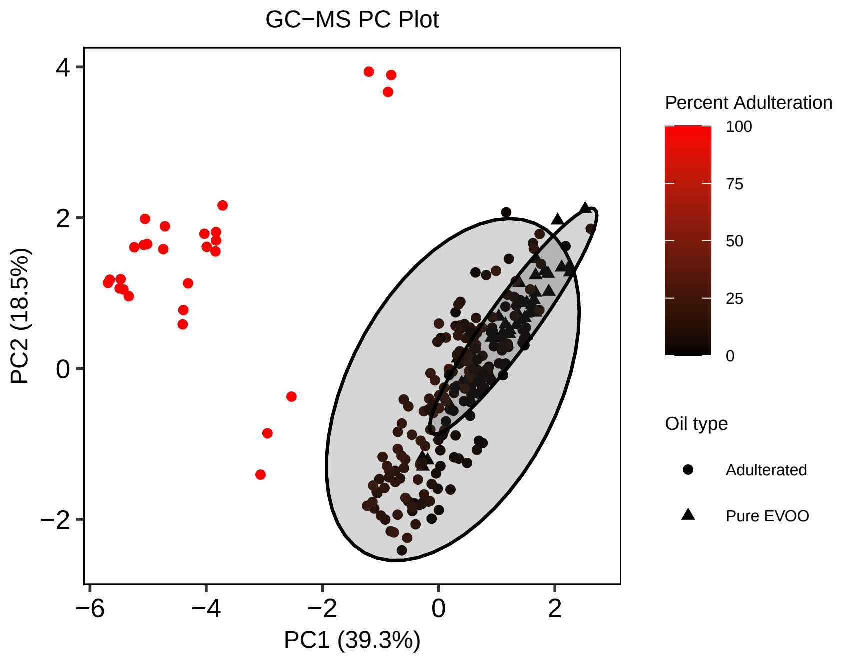
```
#Uv_Vis Plot
p4 <- uvvis_new%>%
  ggplot(mapping = aes(x = PC_1, y = PC_2, shape = class_1, color = perc_adulter)) +
  geom_point() +
  labs(x = "PC1 (74.5%)", y = "PC2 (11.7%)",title = "Uv_Vis PC Plot", shape = "Oil type", color =
  theme_bw() +
  theme(
    panel.border = element_rect(color = 'black', fill = NA),
    panel.grid = element_blank(),
    axis.text.x = element_text(color = 'black', size = 10),
    axis.text.y = element_text(color = 'black', size = 10),
    aspect.ratio = 1,
    axis.title.x = element_text(size = 9),
    axis.title.y = element_text(size = 9),
    plot.title = element_text(size = 9, hjust = 0.5),
    legend.title = element_text(size = 7),
    legend.text = element_text(size = 6)) +
  scale_color_gradient(low = "#000000", high = "red") +
  stat_ellipse(aes(group = class_1),
               level = 0.95,
               geom = "polygon", alpha = 0.2,
               color = 'black', linewidth = 0.6)
```

Patch the PC Plots together

```
suppressWarnings(suppressMessages(library(gridExtra)))
grid.arrange(p1,p2,p3,p4, nrow = 2)
```



```
#GC-MS Plot
p5 <- gc_new %>%
  ggplot(mapping = aes(x = PC_1, y = PC_2, shape = class_1, color = perc_adulter)) +
  geom_point() +
  labs(x = "PC1 (39.3%)", y = "PC2 (18.5%)",title = "GC-MS PC Plot", shape = "Oil type", color =
  theme_bw() +
  theme(
    panel.border = element_rect(color = 'black', fill = NA),
    panel.grid = element_blank(),
    axis.text.x = element_text(color = 'black', size = 10),
    axis.text.y = element_text(color = 'black', size = 10),
    aspect.ratio = 1,
    axis.title.x = element_text(size = 9),
    axis.title.y = element_text(size = 9),
    plot.title = element_text(size = 9, hjust = 0.5),
    legend.title = element_text(size = 7),
    legend.text = element_text(size = 6)) +
  scale_color_gradient(low = "#000000", high = "red") +
  stat_ellipse(aes(group = class_1),
               level = 0.95,
               geom = "polygon", alpha = 0.2,
               color = 'black', linewidth = 0.6)
#Display plot
p5
```



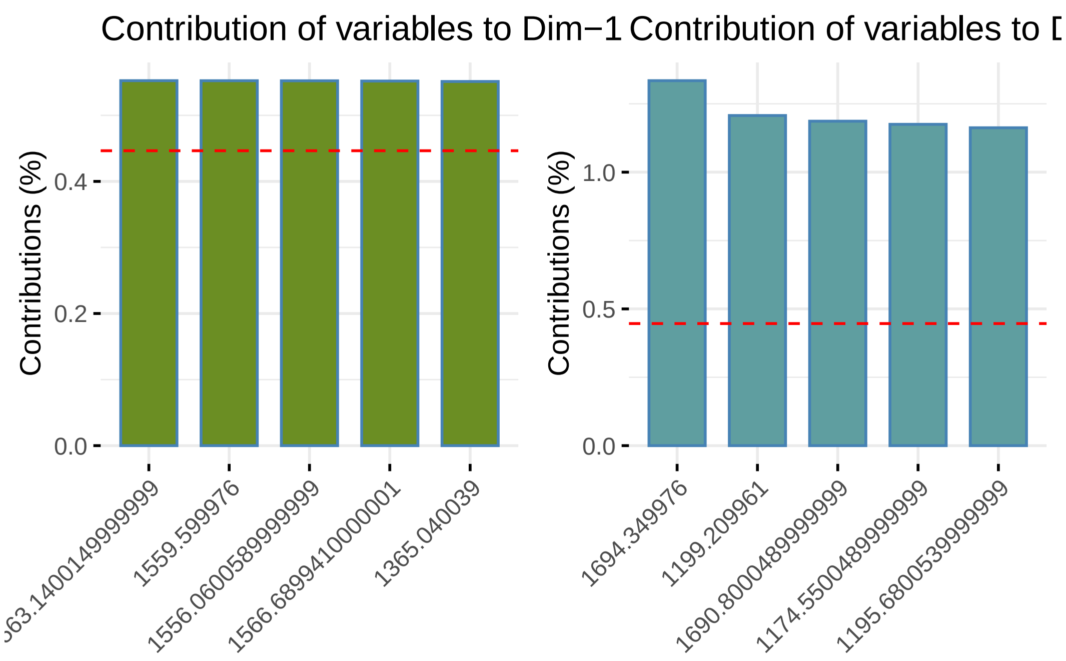
PCA Insights

- PCA results indicate interesting patterns. Although the separation does not appear to be very clear, authentic olive oil tends to separate from adulterated olive oils, especially with HSI, UV-Vis, and GC-MS. PCA, however, demonstrates weakness in discerning oils adulterated at different levels, hence the need for additional supervised algorithms.

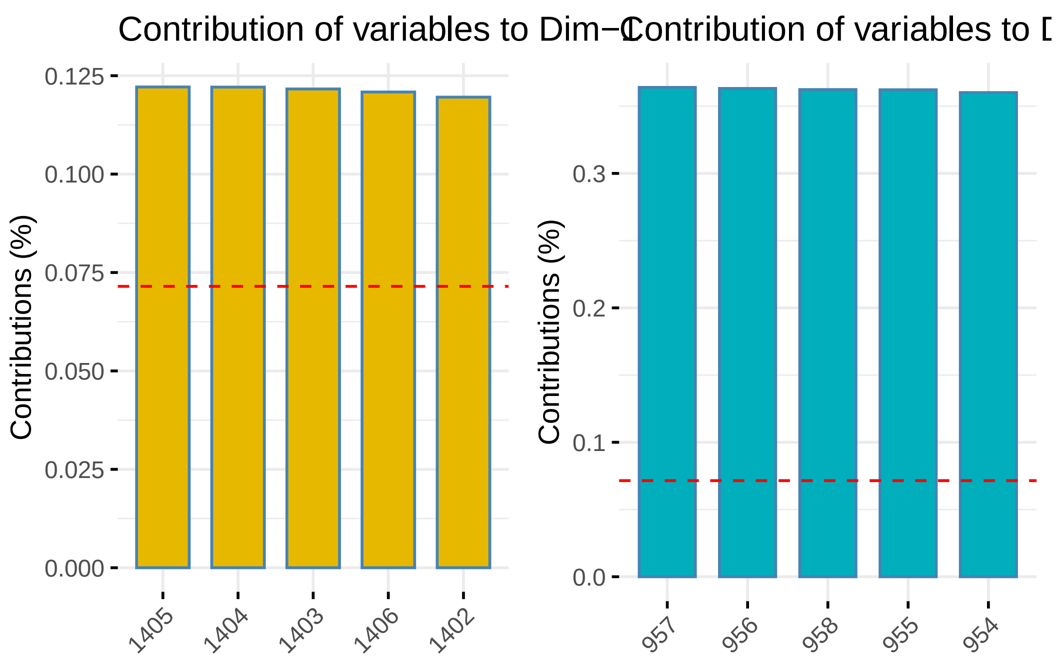
PC variable contributions

This section investigates the contribution of different variables to the variation in principal components (PCs). By analyzing the loadings of each variable on the principal components, we can determine which variables have the most significant impact on the observed patterns in the data. This analysis helps to identify key features that drive the separation of samples in the PCA plot.

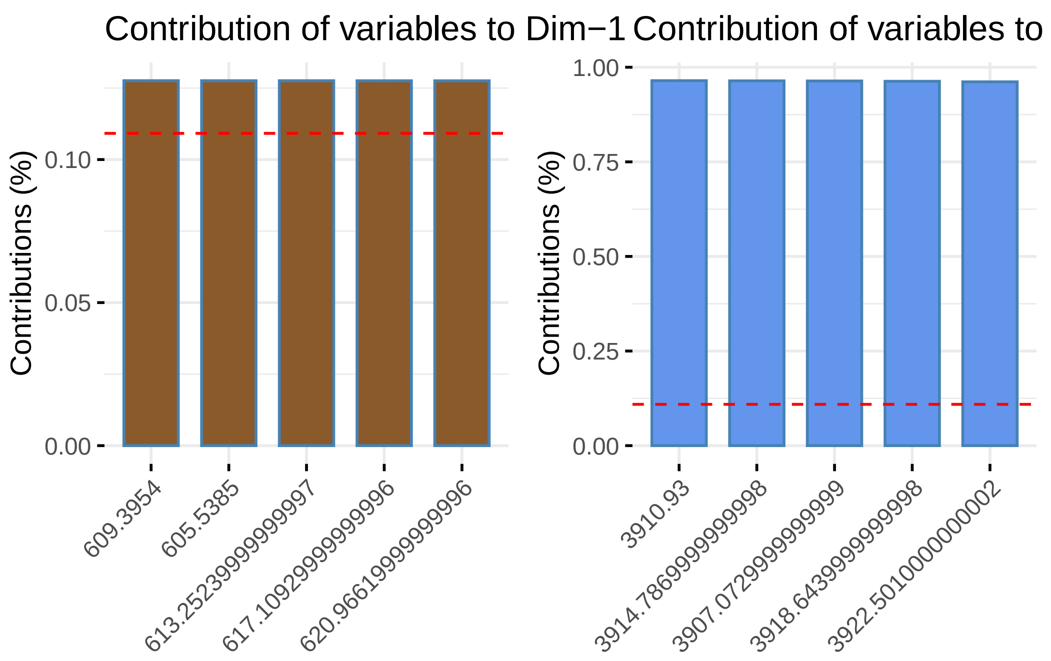
```
#HSI
h1<-fviz_contrib(hsi_pca, choice = "var", top = 5,axes = 1, sort.val = 'desc', fill = "olivedrab"
h2<-fviz_contrib(hsi_pca, choice = "var", top = 5,axes = 2, sort.val = 'desc', fill = "cadetblue"
grid.arrange(h1,h2, nrow = 1)
```



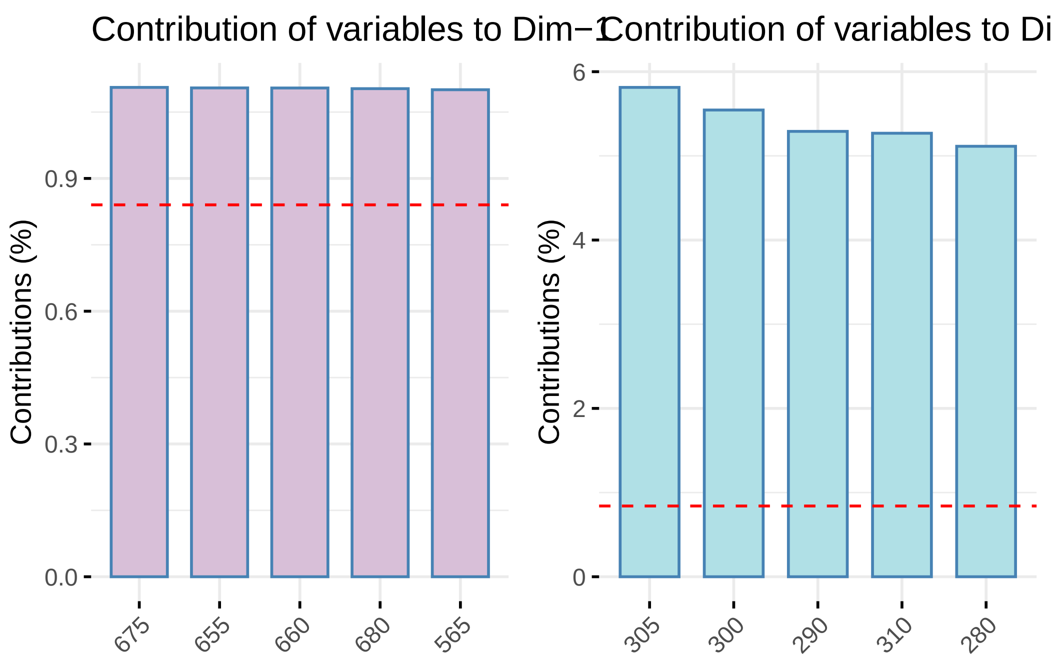
```
#Raman
r1<-fviz_contrib(raman_pca, choice = "var", top = 5,axes = 1, sort.val = 'desc', fill = "#E7B800"
r2<-fviz_contrib(raman_pca, choice = "var", top = 5,axes = 2, sort.val = 'desc', fill = "#00AFBB"
grid.arrange(r1,r2, nrow = 1)
```



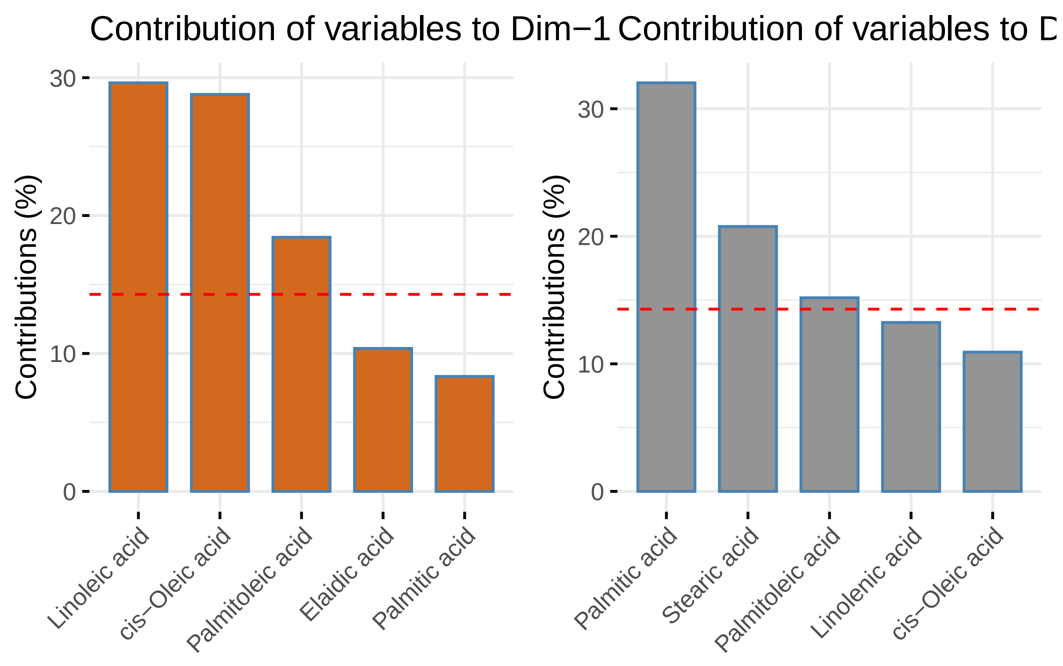
```
#FTIR
f1<-fviz_contrib(ftir_pca, choice = "var", top = 5,axes = 1, sort.val = 'desc', fill = "tan4")
f2<-fviz_contrib(ftir_pca, choice = "var", top = 5,axes = 2, sort.val = 'desc', fill = "cornflowe
grid.arrange(f1,f2, nrow = 1)
```



```
#Uv-Vis
uv1<-fviz_contrib(uv_vis_pca, choice = "var", top = 5,axes = 1, sort.val = 'desc', fill = "thistl
uv2<-fviz_contrib(uv_vis_pca, choice = "var", top = 5,axes = 2, sort.val = 'desc', fill = "powder
grid.arrange(uv1,uv2, nrow = 1)
```



```
#GC-MS
gc1<-fviz_contrib(gc_ms_pca, choice = "var", top = 5,axes = 1, sort.val = 'desc', fill = "chocola
gc2<-fviz_contrib(gc_ms_pca, choice = "var", top = 5,axes = 2, sort.val = 'desc', fill = "gray58"
grid.arrange(gc1,gc2, nrow = 1)
```

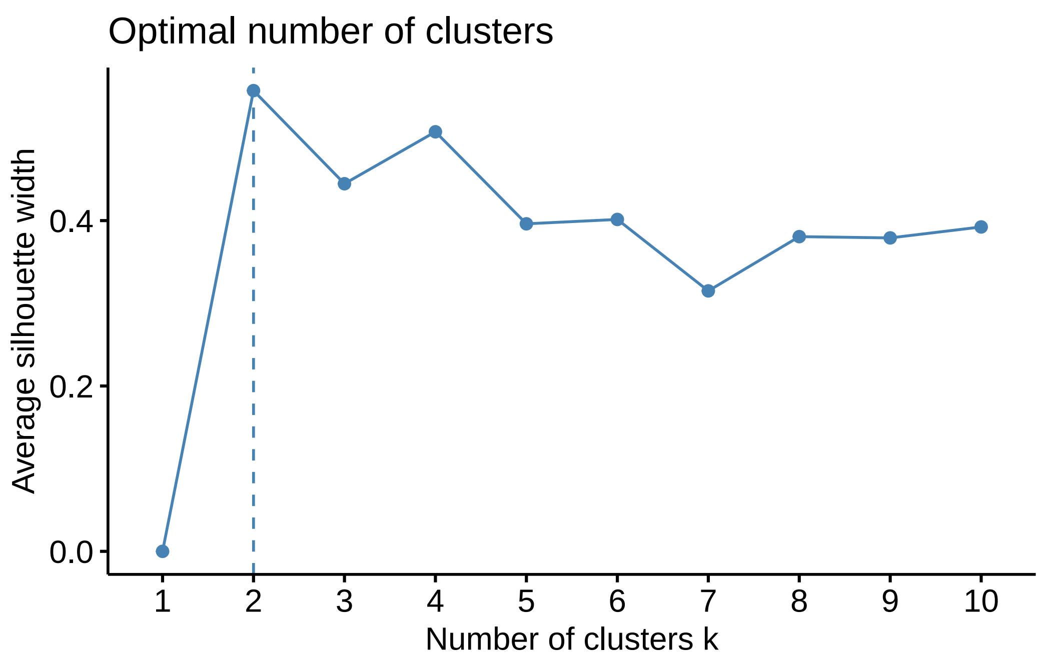


K-Means Clustering

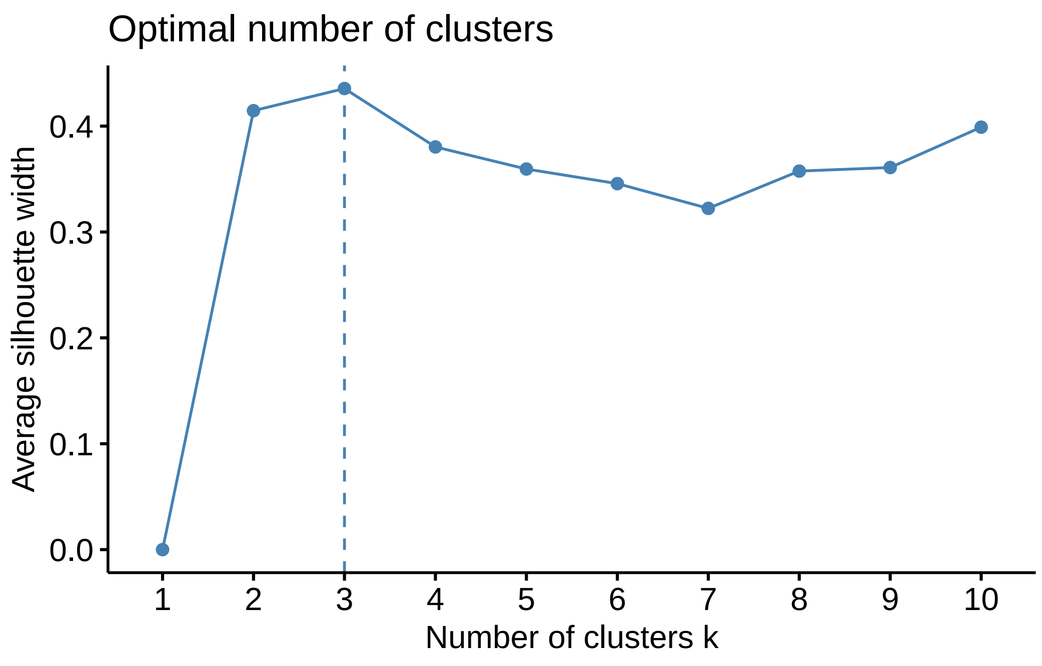
K-means clustering is an unsupervised machine learning algorithm used to partition a dataset into **K distinct, non-overlapping groups** (or clusters) based on feature similarity. It aims to minimize the variance within each cluster and maximize the variance between clusters.

- Let us find the number of **clusters** based on silhoutte method

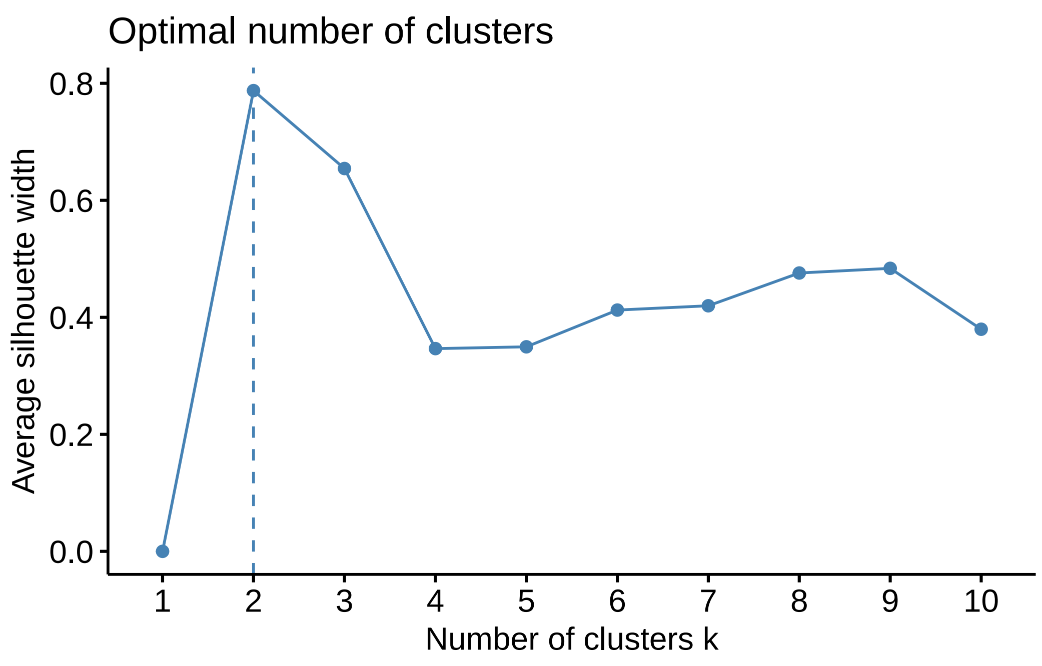
```
# optimal number of clusters for HSI
hsi_clust<-fviz_nbclust(hsi[,-c(1:2)], kmeans, method = "silhouette", k.max=10)
print(hsi_clust)
```



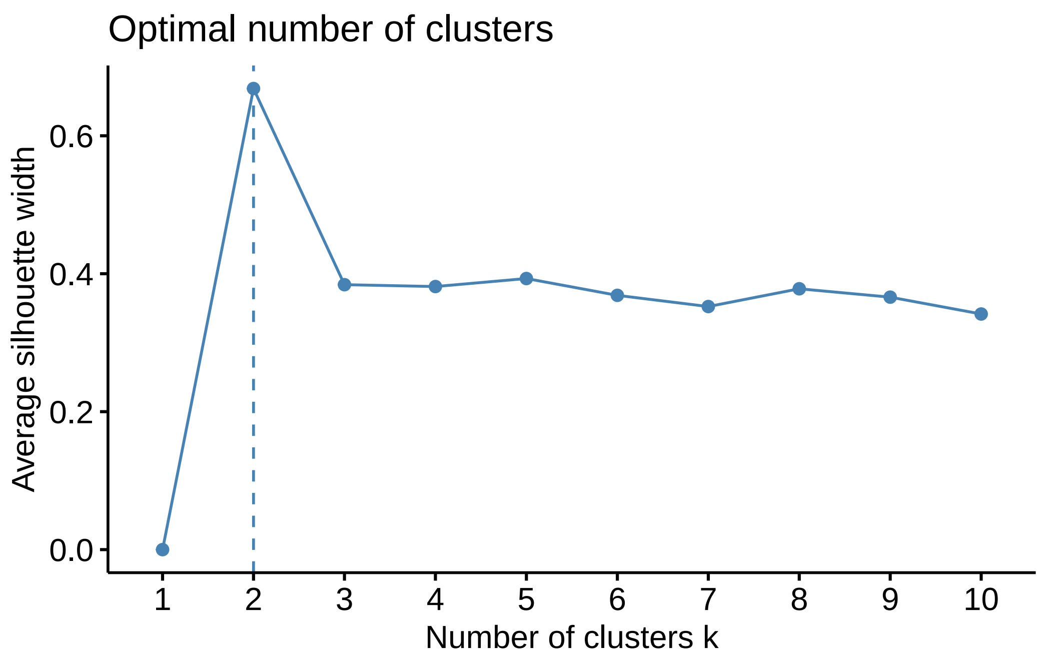
```
# optimal number of clusters for Raman
raman_clust<-fviz_nbclust(raman, kmeans, method = "silhouette", k.max=10)
print(raman_clust)
```



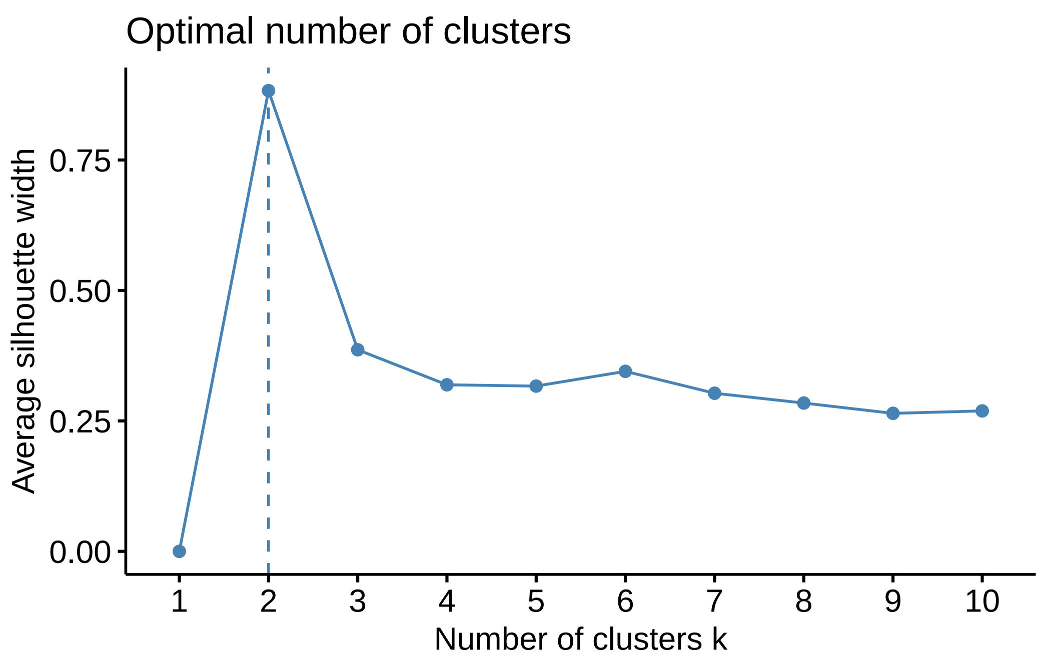
```
#optimal number of clusters for FTIR
ftir_clust<-fviz_nbclust(ftir[,-c(1,2)], kmeans, method = "silhouette", k.max=10)
print(ftir_clust)
```



```
#optimal number of clusters for UV-Vis
uvvis_clust<-fviz_nbclust(uv_vis, kmeans, method = "silhouette", k.max=10)
plot(uvvis_clust)
```

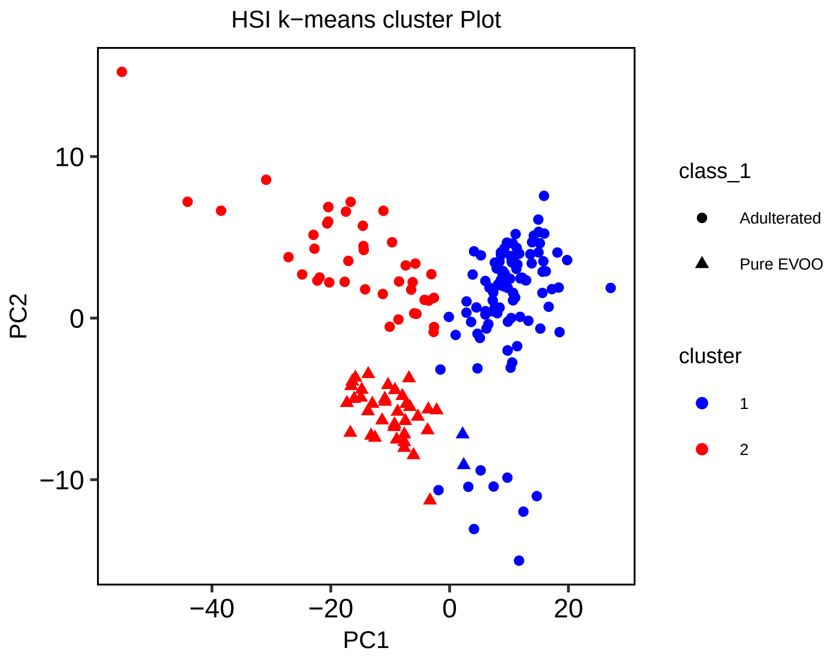


```
#optimal number of clusters for gc-ms
gc_clust<-fviz_nbclust(gc, kmeans, method = "silhouette", k.max=10)
print(gc_clust)
```

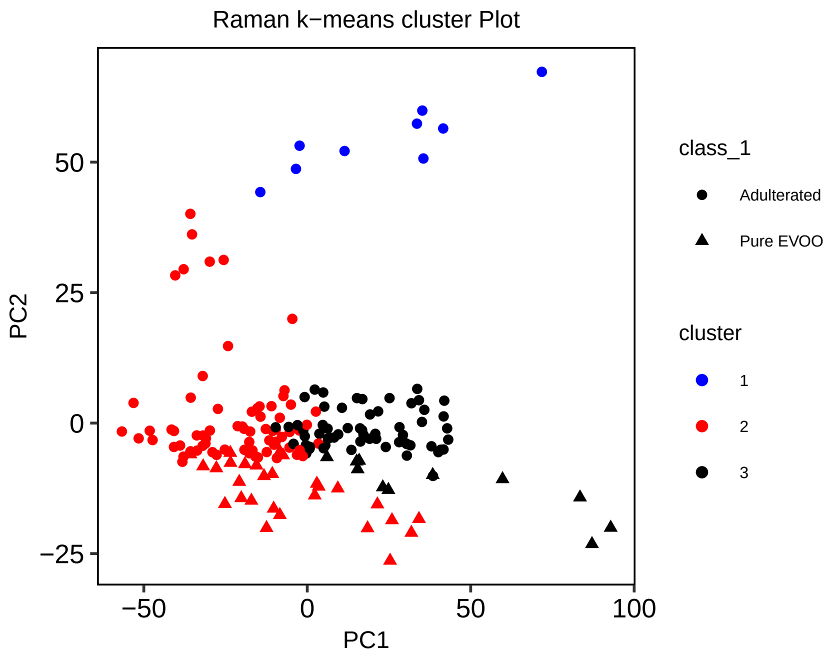


- Then **let us perform k-means clustering with the optimal number of clusters**

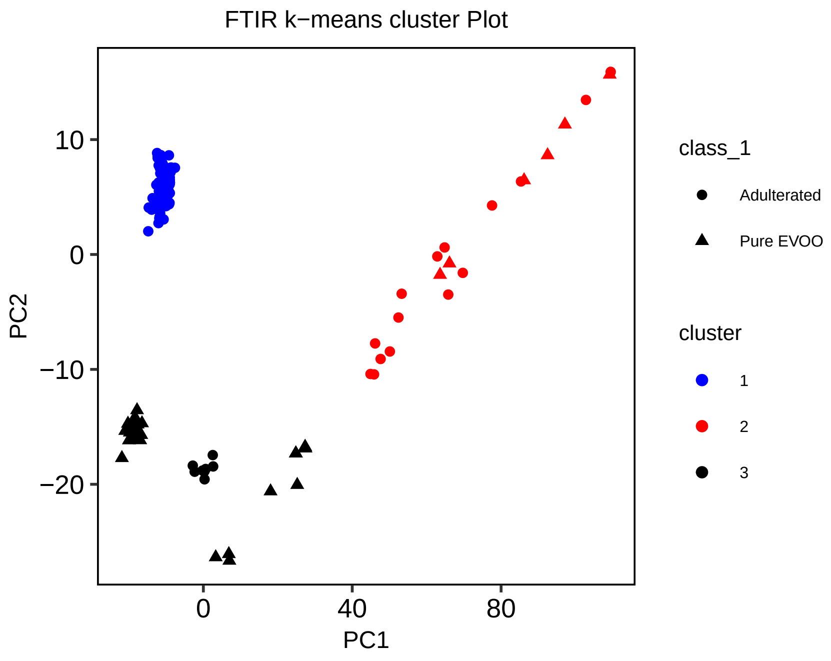
```
#HSI k-means analysis and plots

hsi_kmeans <- kmeans(hsi[,-c(1,2)],2)
cluster<-  hsi_kmeans$cluster
hsi_k_data <-cbind(hsi_new,cluster)
hsi_k_data$cluster<-as.factor(hsi_k_data$cluster)

hsi_k_data %>%
  ggplot(mapping = aes(x = PC_1, y = PC_2, color = cluster, shape = class_1)) +
  geom_point() +
  labs(x = "PC1", y = "PC2",title = "HSI k-means cluster Plot")+
  theme_bw() +
  theme(
    panel.border = element_rect(color = 'black', fill = NA),
    panel.grid = element_blank(),
    axis.text.x = element_text(color = 'black', size = 10),
    axis.text.y = element_text(color = 'black', size = 10),
    aspect.ratio = 1,
    axis.title.x = element_text(size = 9),
    axis.title.y = element_text(size = 9),
    plot.title = element_text(size = 9, hjust = 0.5),
    legend.title = element_text(size = 8),
    legend.text = element_text(size = 6),
    legend.position = "right")+
  scale_color_manual(values = c("blue", "red"))
```



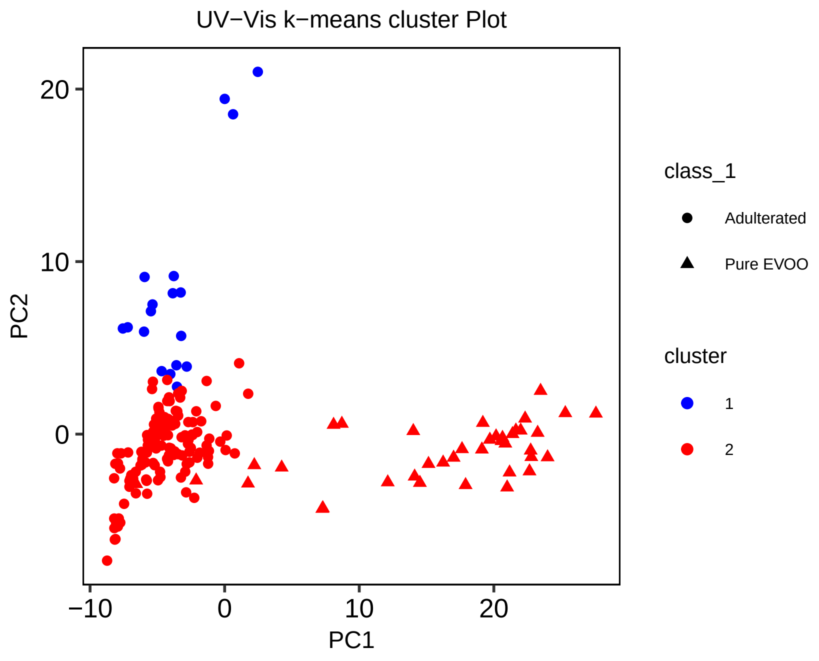
```
#Raman k-means analysis and plotting

raman_kmeans <- kmeans(raman,3)
cluster<-  raman_kmeans$cluster
raman_k_data <-cbind(raman_new,cluster)
raman_k_data$cluster<-as.factor(raman_k_data$cluster)

raman_k_data %>%
  ggplot(mapping = aes(x = PC_1, y = PC_2, color = cluster, shape = class_1)) +
  geom_point() +
  labs(x = "PC1", y = "PC2",title = "Raman k-means cluster Plot")+
  theme_bw() +
  theme(
    panel.border = element_rect(color = 'black', fill = NA),
    panel.grid = element_blank(),
    axis.text.x = element_text(color = 'black', size = 10),
    axis.text.y = element_text(color = 'black', size = 10),
    aspect.ratio = 1,
    axis.title.x = element_text(size = 9),
    axis.title.y = element_text(size = 9),
    plot.title = element_text(size = 9, hjust = 0.5),
    legend.title = element_text(size = 8),
    legend.text = element_text(size = 6),
    legend.position = "right")+
  scale_color_manual(values = c("blue", "red","black"))
```



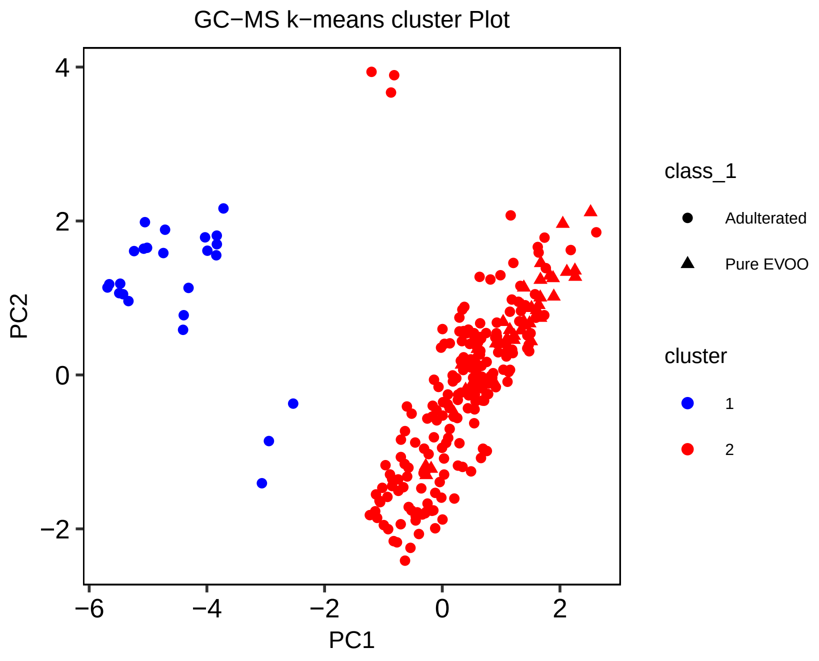
```
#FTIR k-means analysis and plotting

ftir_kmeans <- kmeans(ftir[,-c(1,2)],3)
cluster<-  ftir_kmeans$cluster
ftir_k_data <-cbind(ftir_new,cluster)
ftir_k_data$cluster<-as.factor(ftir_k_data$cluster)

ftir_k_data %>%
  ggplot(mapping = aes(x = PC_1, y = PC_2, color = cluster, shape = class_1)) +
  geom_point() +
  labs(x = "PC1", y = "PC2",title = "FTIR k-means cluster Plot")+
  theme_bw() +
  theme(
    panel.border = element_rect(color = 'black', fill = NA),
    panel.grid = element_blank(),
    axis.text.x = element_text(color = 'black', size = 10),
    axis.text.y = element_text(color = 'black', size = 10),
    aspect.ratio = 1,
    axis.title.x = element_text(size = 9),
    axis.title.y = element_text(size = 9),
    plot.title = element_text(size = 9, hjust = 0.5),
    legend.title = element_text(size = 8),
    legend.text = element_text(size = 6),
    legend.position = "right")+
  scale_color_manual(values = c("blue", "red","black"))
```



```
#UV-Vis k-means analysis and plotting

uvvis_kmeans <- kmeans(uv_vis,2)
cluster<-  uvvis_kmeans$cluster
uvvis_k_data <-cbind(uvvis_new,cluster)
uvvis_k_data$cluster<-as.factor(uvvis_k_data$cluster)

uvvis_k_data %>%
  ggplot(mapping = aes(x = PC_1, y = PC_2, color = cluster, shape = class_1)) +
  geom_point() +
  labs(x = "PC1", y = "PC2",title = "UV-Vis k-means cluster Plot")+
  theme_bw() +
  theme(
    panel.border = element_rect(color = 'black', fill = NA),
    panel.grid = element_blank(),
    axis.text.x = element_text(color = 'black', size = 10),
    axis.text.y = element_text(color = 'black', size = 10),
    aspect.ratio = 1,
    axis.title.x = element_text(size = 9),
    axis.title.y = element_text(size = 9),
    plot.title = element_text(size = 9, hjust = 0.5),
    legend.title = element_text(size = 8),
    legend.text = element_text(size = 6),
    legend.position = "right")+
  scale_color_manual(values = c("blue", "red"))
```



```
#GC-MS k-means analysis and plotting

gc_kmeans <- kmeans(gc,2)
cluster<-  gc_kmeans$cluster
gc_k_data <-cbind(gc_new,cluster)
gc_k_data$cluster<-as.factor(gc_k_data$cluster)

gc_k_data %>%
  ggplot(mapping = aes(x = PC_1, y = PC_2, color = cluster, shape = class_1)) +
  geom_point() +
  labs(x = "PC1", y = "PC2",title = "GC-MS k-means cluster Plot")+
  theme_bw() +
  theme(
    panel.border = element_rect(color = 'black', fill = NA),
    panel.grid = element_blank(),
    axis.text.x = element_text(color = 'black', size = 10),
    axis.text.y = element_text(color = 'black', size = 10),
    aspect.ratio = 1,
    axis.title.x = element_text(size = 9),
    axis.title.y = element_text(size = 9),
    plot.title = element_text(size = 9, hjust = 0.5),
    legend.title = element_text(size = 8),
    legend.text = element_text(size = 6),
    legend.position = "right")+
  scale_color_manual(values = c("blue", "red"))
```



- Based on the findings from k-means clustering, an overlap of clusters for the two expected groups is observed. Unsupervised learning, therefore, is not sufficient for separating pure EVOO from adulterated samples, highlighting the need for supervised classification.

Summary

This section of the project demonstrates how unsupervised learning techniques, particularly PCA and K-Means clustering, can be applied to the complex spectral data obtained from NIR-HSI. These methods provide a powerful way to reduce data complexity and uncover patterns that may not be immediately apparent, laying the groundwork for further classification using supervised machine learning models.

Way Forward to Part 2: Supervised Classification Using Machine Learning

Now that **unsupervised learning** techniques like PCA and K-Means clustering have helped reduce the dimensionality of the Near-Infrared Hyperspectral Imaging (NIR-HSI) data and revealed underlying patterns, the next step is to leverage **supervised classification** methods to develop robust models that can distinguish between **pure and adulterated Extra-Virgin Olive Oil (EVOO)**.