```
# Appendix 3

# Libraries
library(fastICA)
library(pls)

# Setup
dataframe = read.csv2("NIRSpectra.csv")
data = dataframe
data$Viscosity = c()



# Task 1 - Standard PCA
pca = prcomp(data)
# Eigenvalues
λ = pca$sdev^2

# Variation proportions for the different eigenvalues
var_props = λ/sum(λ)*100
barplot(var_props[1:10], ylim=c(0,100), col="forestgreen",
        main="Variation proportions for different eigenvalues",
        xlab="λi", ylab="Varaible proportion") # The plot shows that 2 PCs should be extracted
sum(var_props[1:2]) #= 99.5957 --> PC1 and PC2 count for 99.5957% of the variation

# Scores - There seems to be least 2 unusual diesiel fuels according to this plot
plot(pca$x[,1], pca$x[,2], xlab="PC1", ylab="PC2", main="Projected Values, PCA") # 2 "strong" outliers, 5-7 "medium"
outliers



# Task 2 - Trace Plots
U = pca$rotation # projected values

# Tracing plots
plot(U[,1], main="Traceplot for PC1", ylim=c(-0.11,0.11), ylab="Projection/Rotation Value")
plot(U[,2], main="Traceplot for PC2", ylim=c(-0.3, 0.3), ylab="Projection/Rotation Value") # the last few original
feutures mainly explain this PC



# Task 3 - ICA
set.seed(12345)
ica = fastICA(data, 2, alg.typ="parallel", fun="logcosh", alpha=1, method="R", row.norm=FALSE, maxit=200, tol=0.0001,
verbose=TRUE)
Wtick = ica$K%*%ica$W
plot(Wtick[,1], main="Traceplot, W' column 1", ylim=c(-1, 1), ylab="Projection/Rotation Value")
plot(Wtick[,2], main="Traceplot, W' column 2", ylim=c(-11,11), ylab="Projection/Rotation Value") # the "opposite" to
PCA, similar information

# Scores
plot(ica$S[,1], ica$S[,2], xlab="Z1", ylab="Z2", main="Projected Values, ICA") # ICA,



# Task 4 - PCR
set.seed(12345)
pcr = pcr(Viscosity~., data=dataframe, validation="CV")
validationplot(pcr, val.type="MSEP", main="Dependence of MSEP (Mean Squared Error of Prediction) and #components")
```