Machine Learning - Block 2 Assignment 2

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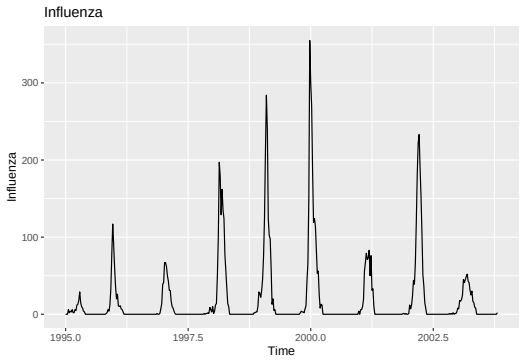
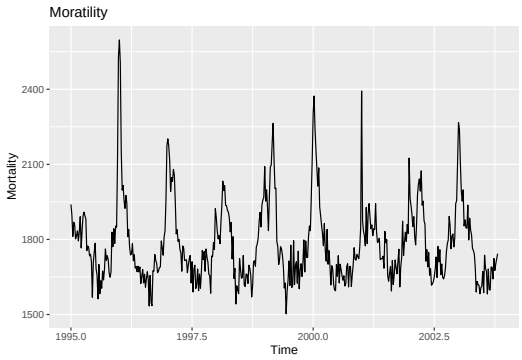
Assignment 1. Using GAM and GLM to examine mortality rates

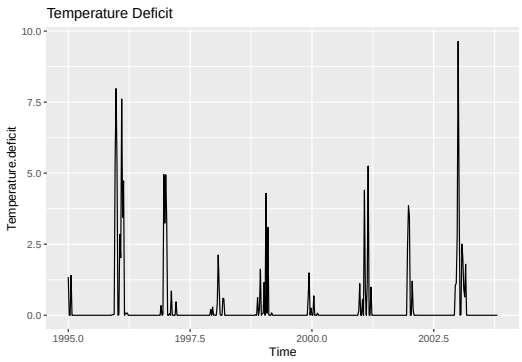
The Excel document influenza.xlsx contains weekly data on the mortality and the number of laboratory-confirmed cases of influenza in Sweden. In addition, there is information about population-weighted temperature anomalies (temperature deficits).

1. Use time series plots to visually inspect how the mortality and influenza number vary with time (use Time as X axis). By using this plot, comment how the amounts of influenza cases are related to mortality rates.

Plotting the data against the time:

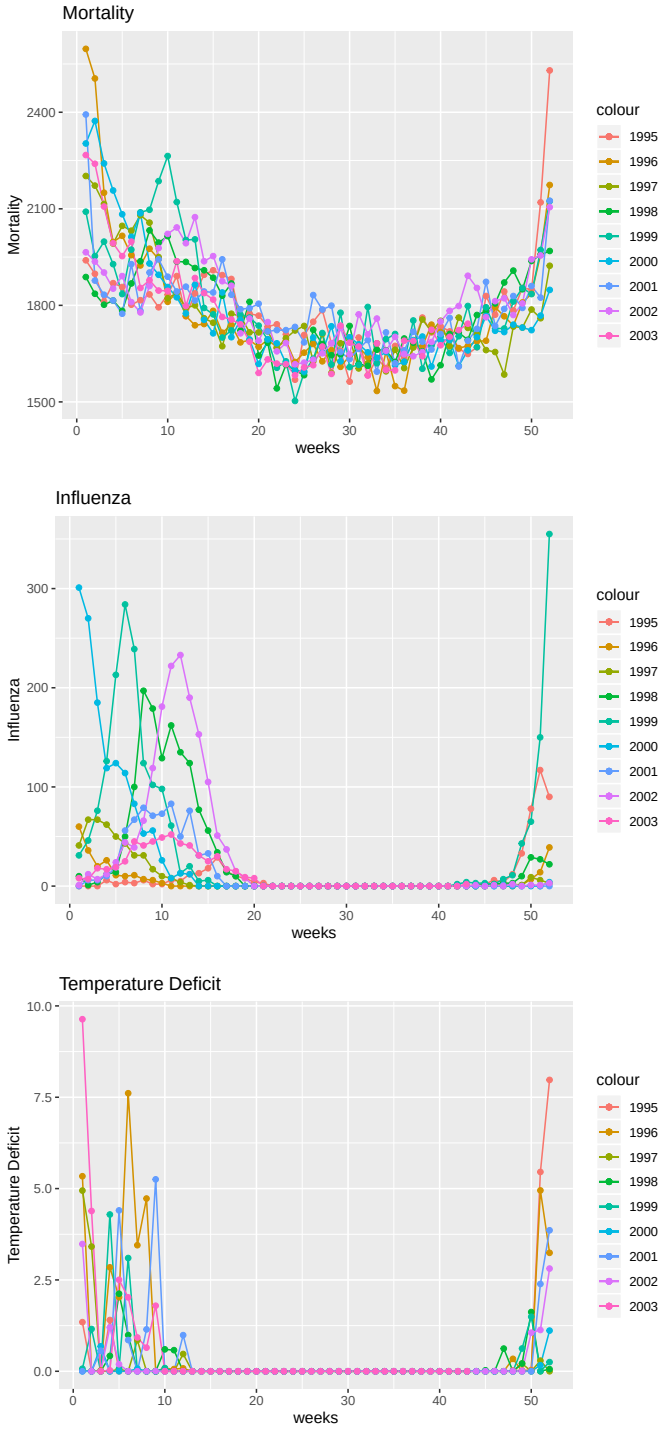






It seems to be a modality in the data. It can be seen that Influenza peaks seems to have a correlation with peaks in mortality and temperature deficit

As the model is meant to learn from weeks variations along the year, it is better to separate the data into several time series per year and see how the data looks now.



Now it is quite clear that the data shows that during winter weeks Influenza cases and Mortality related to increases, also the temperature deficit seems to follow that trend.

2. Use gam() function from mgcv package to fit a GAM model in which Mortality is normally distributed and modelled as a linear function of Year and spline function of Week, and make sure that the model parameters are selected by the generalized cross-validation. Report the underlying probabilistic model.

It is fitted one model with the following formula:

$$Mortality \approx Year + spline(Week)$$

The summary of the obtained probabilistic model is:

```
##
## Family: gaussian
## Link function: identity
##
## Formula:
## Mortality ~ Year + s(Week, k = length(unique(data$Week)))
##
## Parametric coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) -680.598   3367.760  -0.202    0.840
## Year           1.233      1.685   0.732    0.465
##
## Approximate significance of smooth terms:
##           edf Ref.df     F p-value
## s(Week) 14.32  17.87 53.86  <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Rank: 52/53
## R-sq.(adj) =  0.677   Deviance explained = 68.8%
## GCV = 8708.6  Scale est. = 8398.9    n = 459
```

The model Mean and variance are :

```
## [1] "Train predictions mean:"
```

```
## [1] 1783.765
```

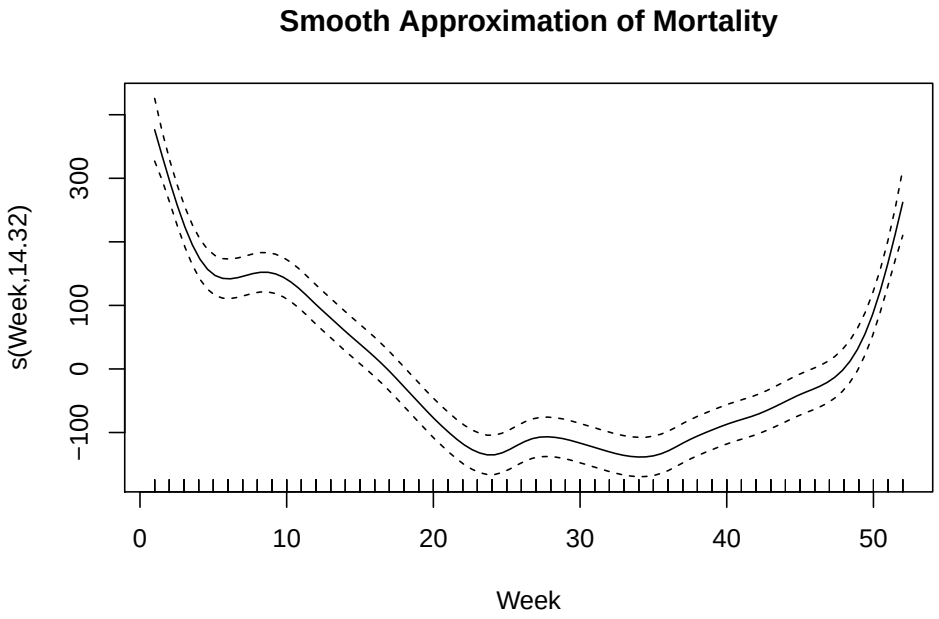
```
## [1] "Train predictions variance:"
```

```
## [1] 25981.62
```

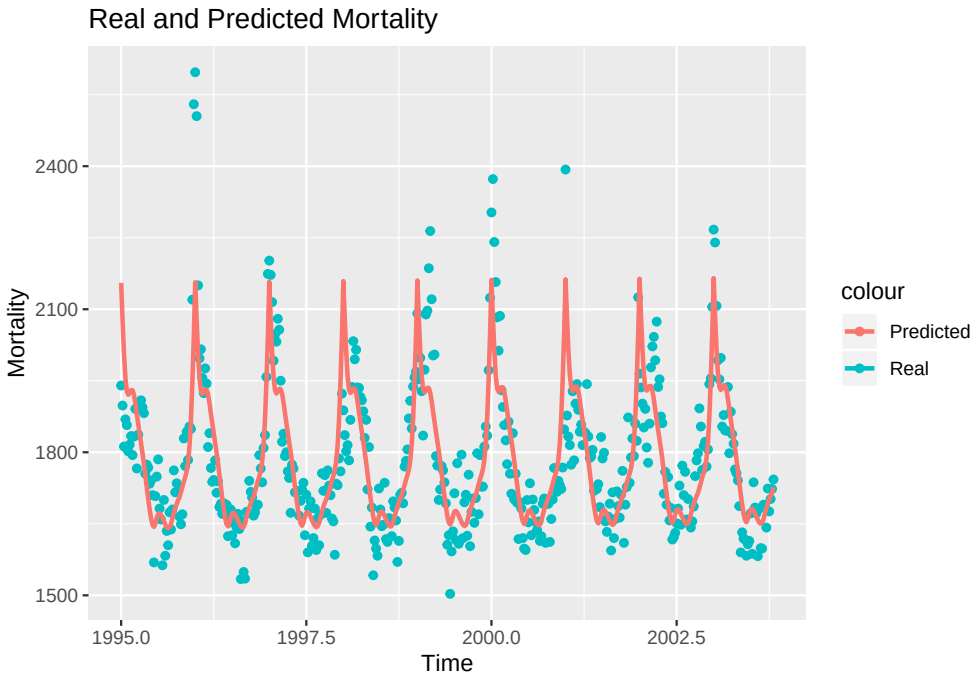
Thus as the summary states that the model family is Gaussian, it can be said that :

$$Mortality \sim Year + spline(Week)$$
$$Mortality \sim N(\mu = 1783.765, \sigma = 25981.62)$$

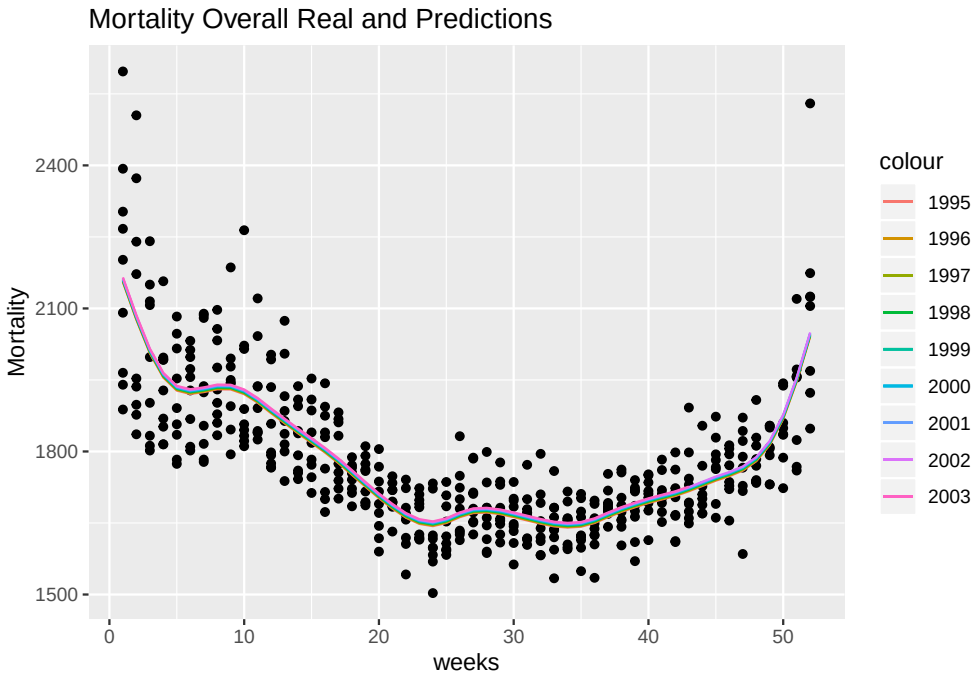
The smoother curve approximated by the GAM model is:



3. Plot predicted and observed mortality against time for the fitted model and comment on the quality of the fit. Investigate the output of the GAM model and report which terms appear to be significant in the model. Is there a trend in mortality change from one year to another? Plot the spline component and interpret the plot.



Although it seems to be a fair general approximation it seems to be missing some abnormal positive and negative peaks.



It can be seen that given the variability of mortality per week each year, the GAM fit acceptably well the data, though still too general, thus not as good as we would like to.

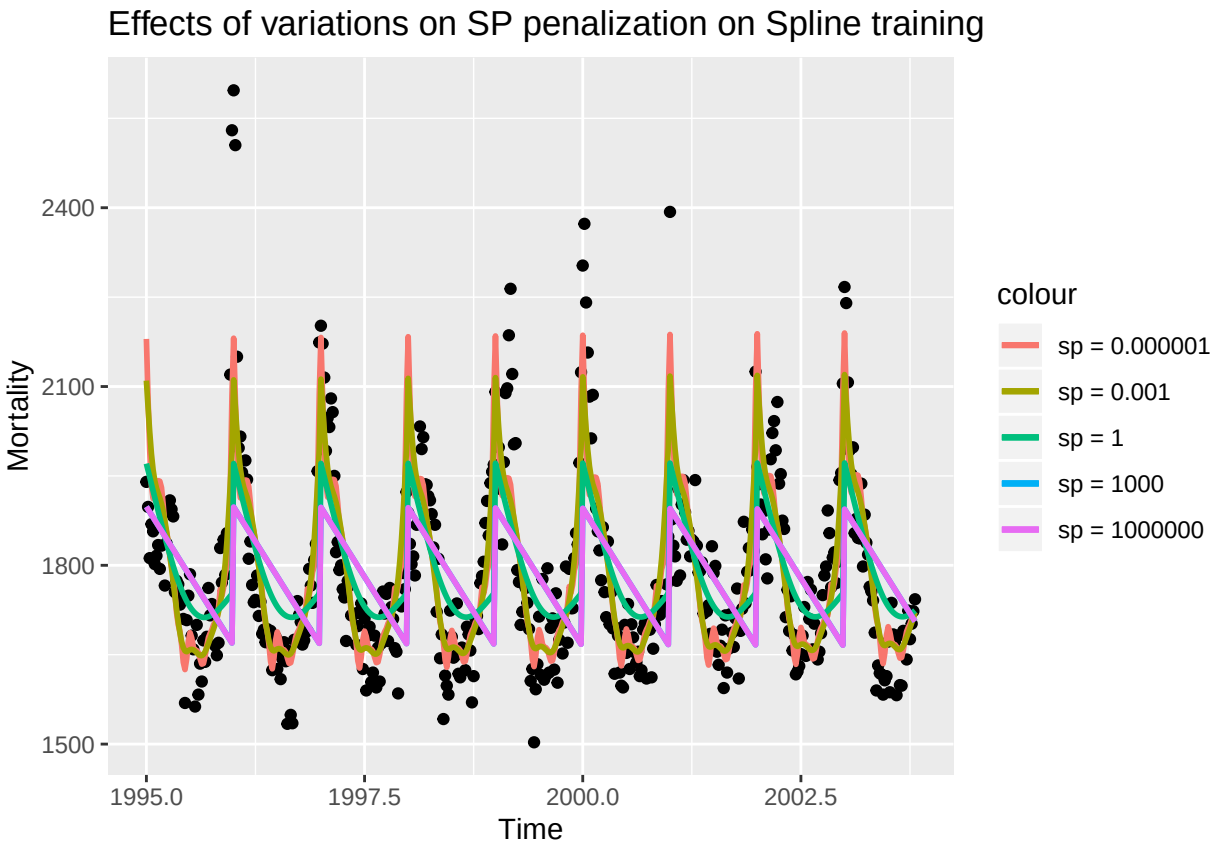
The 10 most significant terms in the model are:

```
## [1] "The 10 most important coefficients:"
```

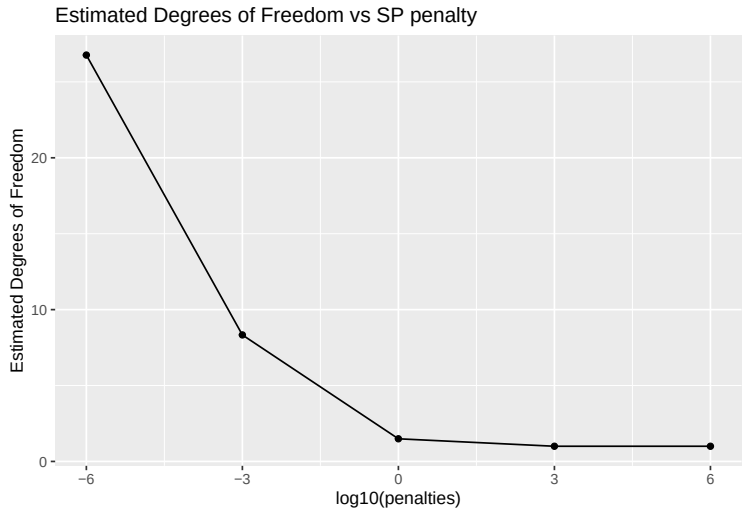
```
## s(Week).26 s(Week).36 s(Week).25 s(Week).20 s(Week).22 s(Week).39 s(Week).18
##   6962.757   6367.777   6224.849   3619.108   2193.085   2038.668   1588.405
## s(Week).16 s(Week).40 s(Week).12
##   1478.684   1468.447   1406.513
```

4. Examine how the penalty factor of the spline function in the GAM model from step 2 influences the estimated deviance of the model. Make plots of the predicted and observed mortality against time for cases of very high and very low penalty factors. What is the relation of the penalty factor to the degrees of freedom? Do your results confirm this relationship?

The smoothing penalty in `gam()` is given by the `sp` parameter sent to the constructor to be used in training. For this testing purpose it have been used the following penalties $\{10^{-6}, 10^{-3}, 1, 10^{3}, 10^{6}\}$



It can be seen that the lower the penalty the better the fit. In this case it looks good to have such a low penalty, though in other cases it might overfit the data.

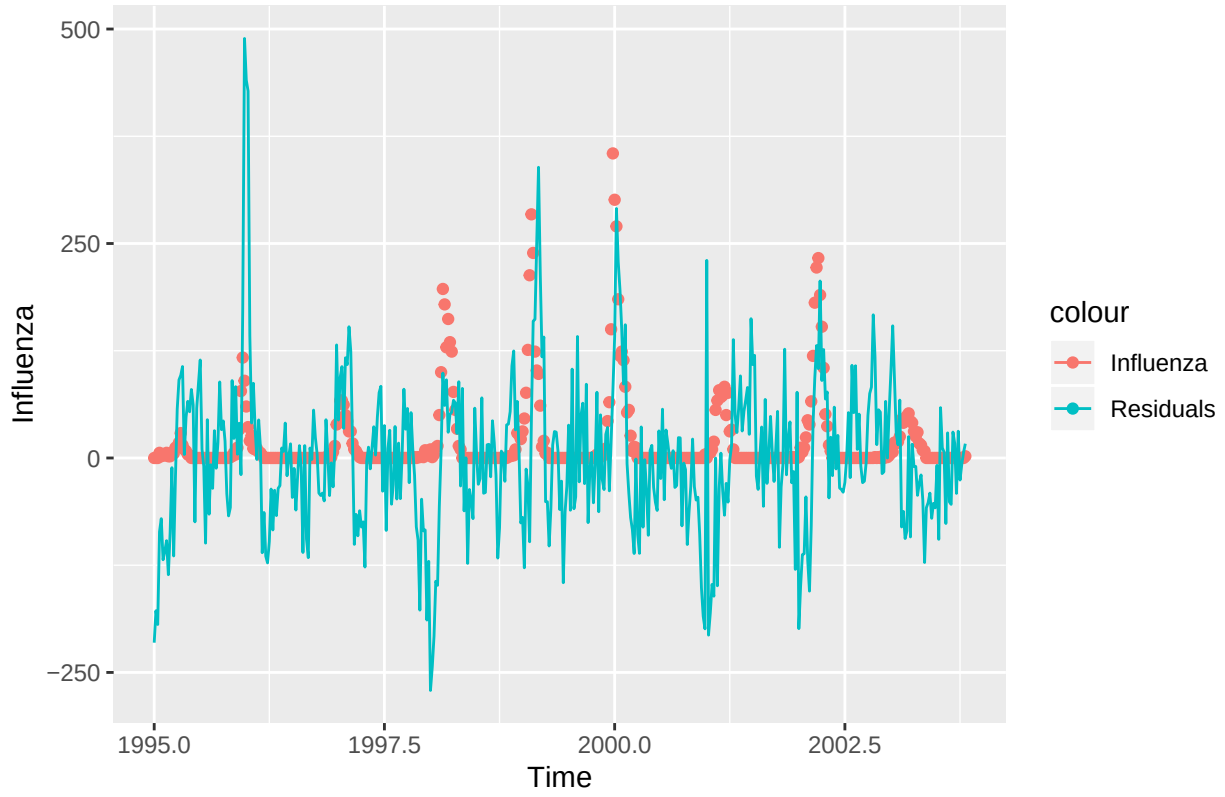


Extracting the degrees of freedom from each penalization iteration it can be seen that the lower the penalization the more relaxed is the model, thus, the higher the degrees of freedom. The penalty factor is inversely proportional to the degrees of freedom. Indeed, by looking at the above plots, this relationship is confirmed. A high penalty essentialy drops a higher number of parameters in the linear smoother matrix S_λ (by approximating them to zero).

5. Use the model obtained in step 2 and plot the residuals and the influenza values against time (in one

plot). Is the temporal pattern in the residuals correlated to the outbreaks of influenza?

At a first glance Residuals seem to be noise compared to Influenza behavior.



Nonetheless visual assumptions might be incorrect. Testing numerically by getting their correlation statistic is low, thus there is no evidence to say that the residuals from the model and the influenza measures are correlated.

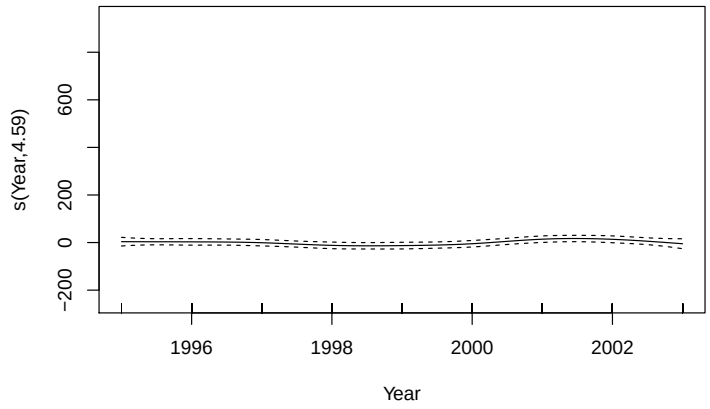
```
## [1] 0.3397395
```

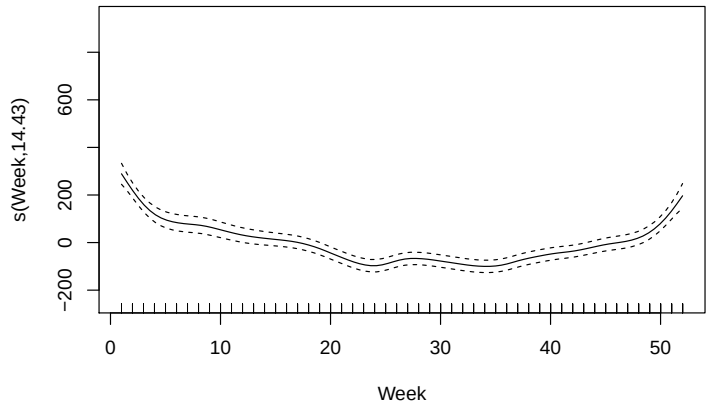
6. Fit a GAM model in R in which mortality is be modelled as an additive function of the spline functions of year, week, and the number of confirmed cases of influenza. Use the output of this GAM function to conclude whether or not the mortality is influenced by the outbreaks of influenza. Provide the plot of the original and fitted Mortality against Time and comment whether the model seems to be better than the previous GAM models.

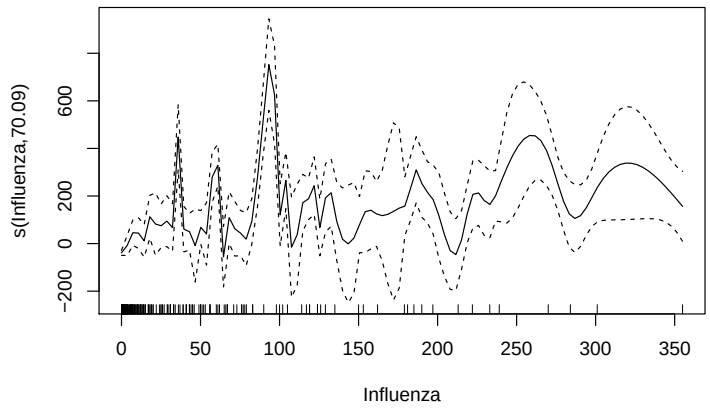
It has been trained a GAM using the following formula:

$$Mortality \approx spline(Year) + spline(Week) + spline(Influenza)$$

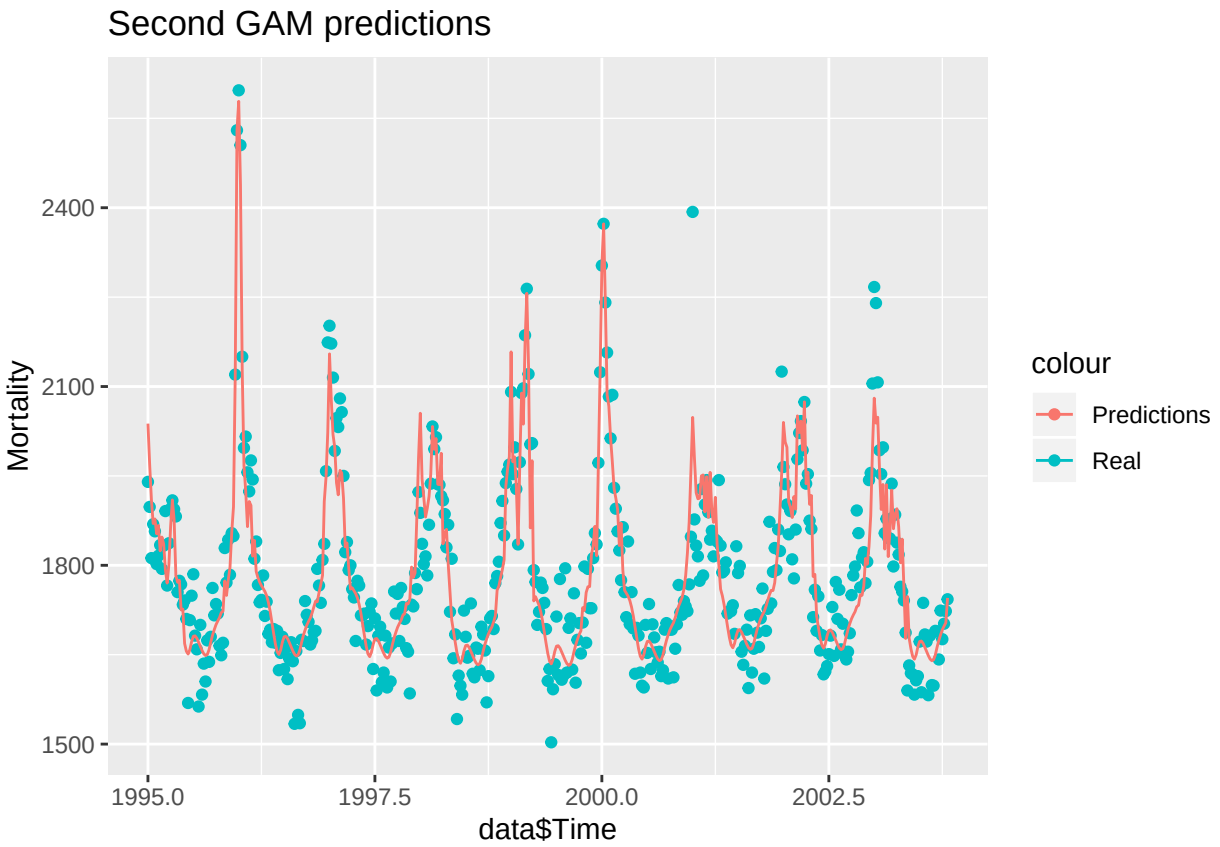
The obtained smoothers are the following.







Now, using the model to predict the Mortality :

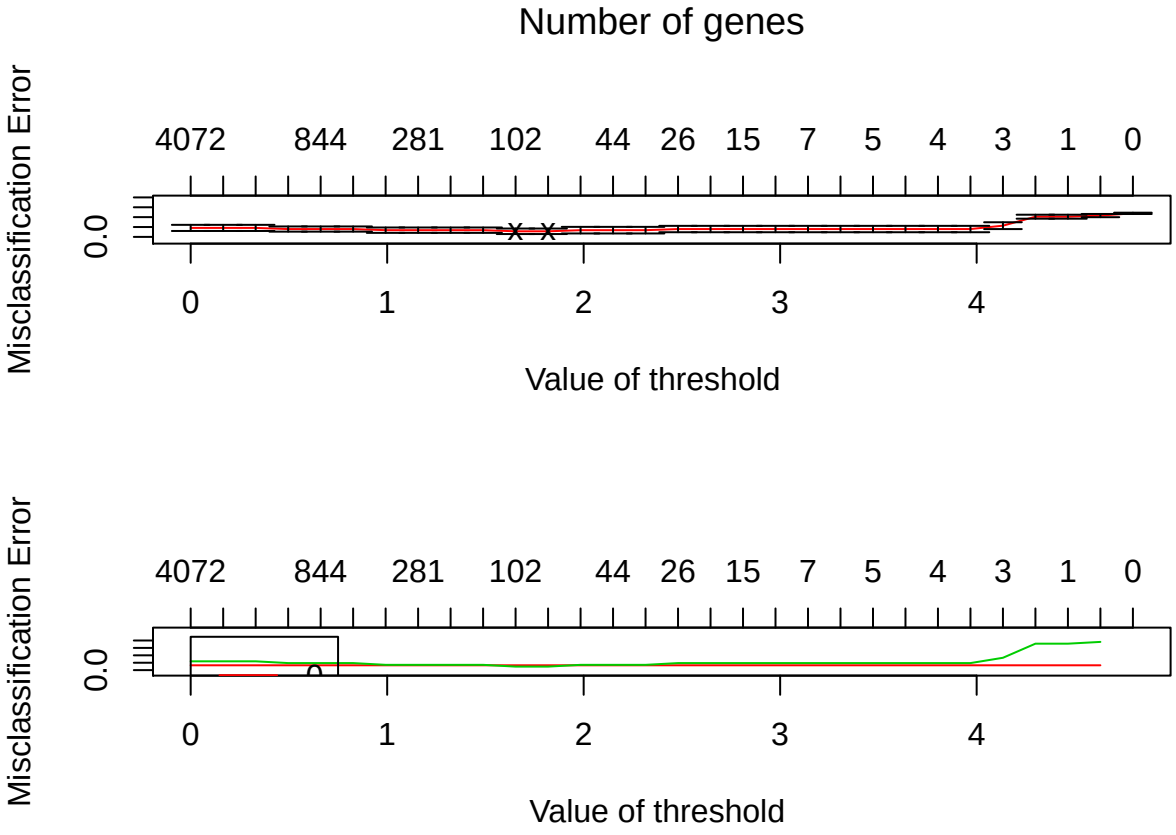


The model seems to fit better the data, though there are still some data points not being well approximatted. This is sign that the predictor is not overfitted, so compared against the previous predictors, this is the best one.

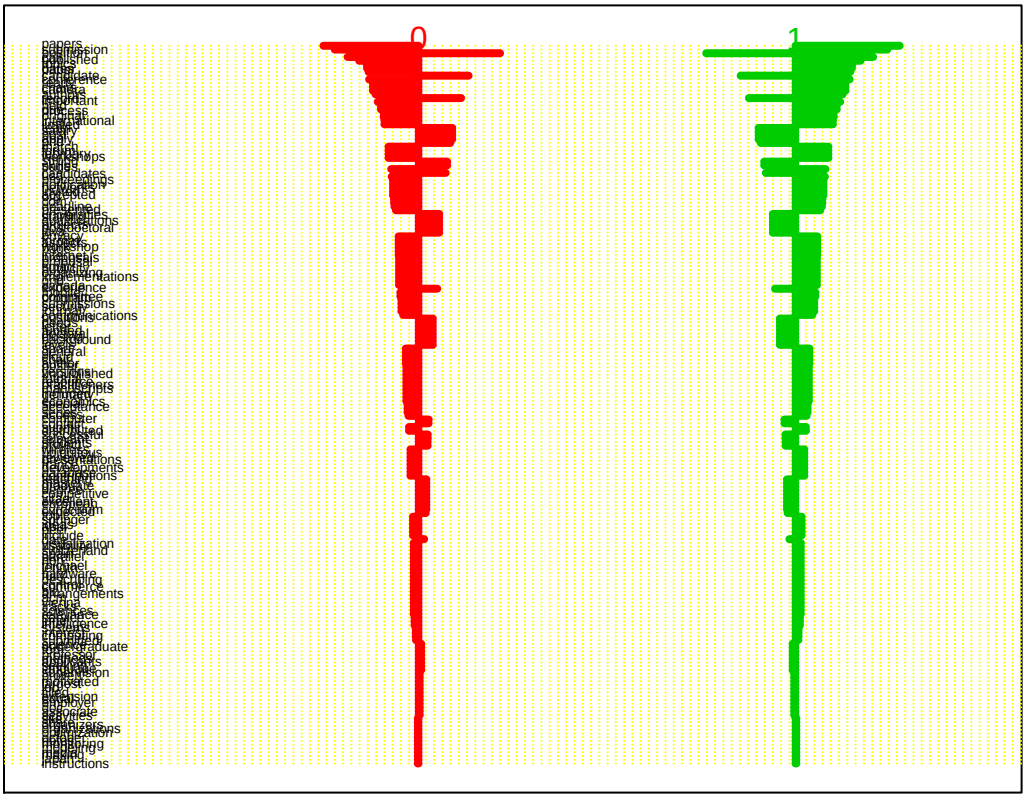
Assignment 2. High-dimensional methods

The data file data.csv contains information about 64 e-mails which were manually collected from DBWorld mailing list. They were classified as: 'announces of conferences' (1) and 'everything else' (0) (variable Conference)

1. Divide data into training and test sets (70/30) without scaling. Perform nearest shrunken centroid classification of training data in which the threshold is chosen by cross-validation. Provide a centroid plot and interpret it. How many features were selected by the method? List the names of the 10 most contributing features and comment whether it is reasonable that they have strong effect on the discrimination between the conference mails and other mails? Report the test error.



Therefore from the crossvalidation results it can be seen that the best performance error-wise is obtained for threshold = 1.29.

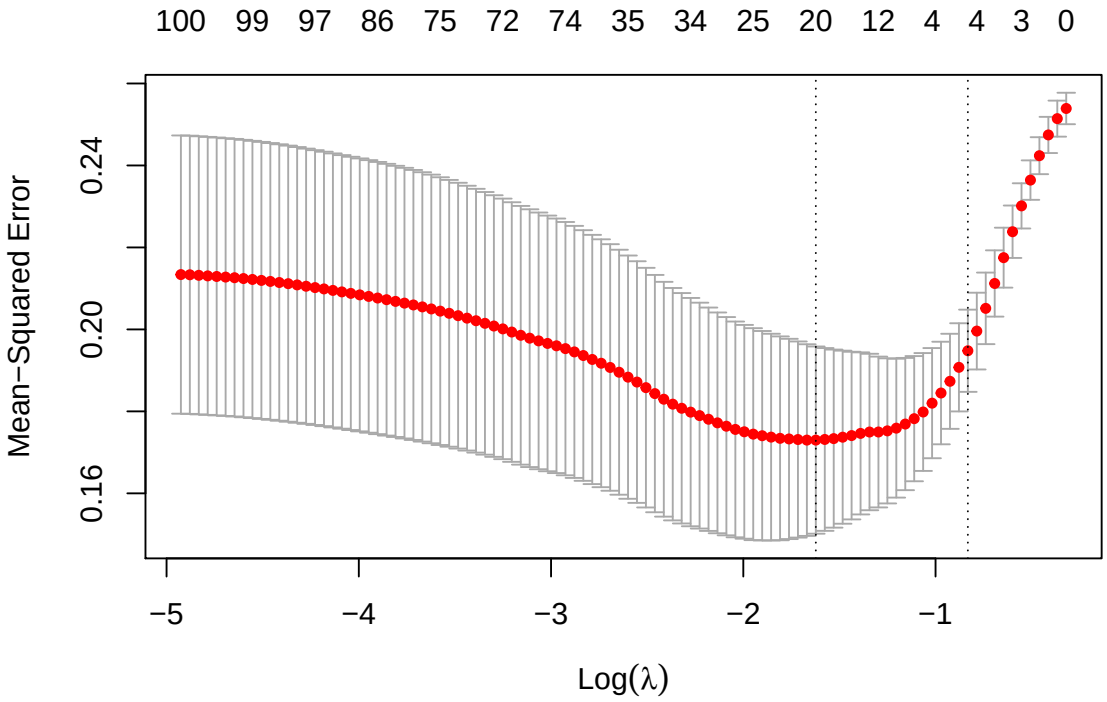



```
## There were selected, 193 features

## [1] "The best 10 selected features are:"

##       id     name         0-score   1-score
##  [1,] "3036" "papers"     "-0.5049" "0.553"
##  [2,] "4060" "submission" "-0.445"  "0.4874"
##  [3,] "3187" "position"   "0.4325"  "-0.4737"
##  [4,] "596"  "call"       "-0.3766" "0.4124"
##  [5,] "3364" "published"  "-0.3153" "0.3453"
##  [6,] "4282" "topics"     "-0.2756" "0.3018"
##  [7,] "1045" "dates"      "-0.2737" "0.2998"
##  [8,] "3035" "paper"      "-0.2655" "0.2907"
##  [9,] "606"  "candidate"  "0.2654"  "-0.2907"
## [10,] "869"  "conference" "-0.2625" "0.2875"

## Classification Performance : Shrunken centroid and shit
## [1] "Confusion Matrix"
##        predictions
## targets  0  1
##       0 12  0
##       1  1  7
## Rates details:
##  TPR = 100 % - TNR = 92.30769 % - FPR = 0 % - FNR = 7.692308 %
##  Misclassification Rate =  5 %
```

2. Compute the test error and the number of the contributing features for the following methods fitted to the training data:

Compare the results of these models with the results of the nearest shrunken centroids (make a comparative table). Which model would you prefer and why?

a. Elastic net with the binomial response and $\alpha = 0.5$ in which penalty is selected by the cross-validation




```
## Classification Performance : ElasticNet
## [1] "Confusion Matrix"
##         predictions
## targets  0  1
##       0 12  0
##       1  2  6
## Rates details:
##  TPR = 100 % - TNR = 85.71429 % - FPR = 0 % - FNR = 14.28571 %
##  Misclassification Rate =  10 %
```

```
## Elasticnet model has  27  nonzero coefficients
```

b. Support vector machine with "vanilladot" kernel.

```
##  Setting default kernel parameters
```

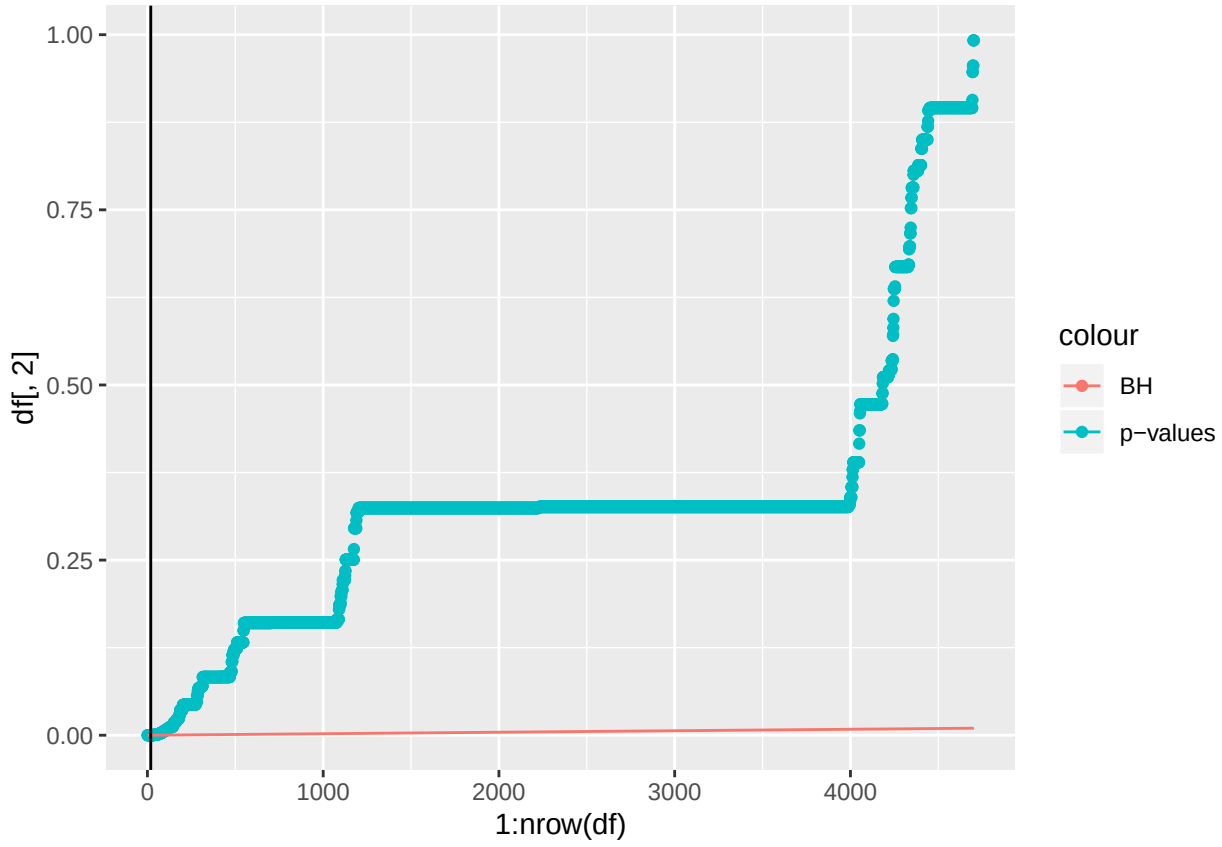
```
## Warning in .local(x, ...): Variable(s) `' constant. Cannot scale data.
```

```
## Classification Performance : SVM - Testing performance
## [1] "Confusion Matrix"
##        predictions
## targets  0  1
##       0 12  0
##       1  1  7
## Rates details:
##  TPR = 100 % - TNR = 92.30769 % - FPR = 0 % - FNR = 7.692308 %
##  Misclassification Rate =  5 %
```

SVMs do not suffer the problem of highdimensional data, it will use all the features to compute the support vectors and the hyperplane fitted by them.

Between Elasticnet and SVM models, the last one performs better.

3. Implement Benjamini-Hochberg method for the original data, and use t.test() for computing p-values. Which features correspond to the rejected hypotheses? Interpret the result.




```
## Rejected Features = 19
##  Rejected Hypothesis Features =
```

```
##  ( 1 ) papers
##  ( 2 ) submission
##  ( 3 ) position
```

```
##  ( 4 ) published
##  ( 5 ) important
##  ( 6 ) call
##  ( 7 ) conference
##  ( 8 ) candidates
##  ( 9 ) dates
##  ( 10 ) paper
##  ( 11 ) topics
##  ( 12 ) limited
##  ( 13 ) candidate
##  ( 14 ) camera
##  ( 15 ) ready
##  ( 16 ) authors
##  ( 17 ) phd
##  ( 18 ) projects
##  ( 19 ) org
```

Appendix A : Environment setup Code

```
knitr::opts_chunk$set(echo = FALSE)
library(openxlsx)
library(ggplot2)
library(mgcv)
library(akima)
library(plotly)
library(pamr)
library(glmnet)
library(e1071)
library(kernlab)
library(readr)
# RNGversion('3.5.1')
set.seed(12345)
```

Appendix B : Code for Assignment 1

```
################################################################################
##                                Assignment 1
################################################################################

# Import data
dataPath <- "data/influenza.xlsx"
data <- read.xlsx(dataPath)

# Time Series plotting
mortPlot <- ggplot(data) +
    geom_line(aes(x=Time, y=Mortality), color="black") + ggtitle("Moratility")
infPlot <- ggplot(data) +
    geom_line(aes(x=Time, y=Influenza), color="black") + ggtitle("Influenza")
tempPlot <- ggplot(data) +
    geom_line(aes(x=Time, y=Temperature.deficit), color="black") +
    ggtitle("Temperature Deficit")
infPlot
mortPlot
tempPlot

# Time series per year
years <- unique(data$Year)
weeks <- unique(data$Week)
mortData <- list()
infData  <- list()
tempData <- list()
for(i in 1:length(years)) {
    year <- years[i]
    mortData[[i]] <- data$Mortality[which(data$Year == year)]
    infData[[i]]  <- data$Influenza[which(data$Year == year)]
    tempData[[i]] <- data$Temperature.deficit[which(data$Year == year)]
}
names(mortData) <- years
names(infData)  <- years
names(tempData) <- years

# create data.frames for ggplot
plotData <- function(d, title) {
    shortWeeks <- 1:length(d$'2003')
    p <- ggplot() +
        geom_line(aes(x=weeks, y=d$'1995', color="1995")) +
        geom_line(aes(x=weeks, y=d$'1996', color="1996")) +
        geom_line(aes(x=weeks, y=d$'1997', color="1997")) +
        geom_line(aes(x=weeks, y=d$'1998', color="1998")) +
        geom_line(aes(x=weeks, y=d$'1999', color="1999")) +
        geom_line(aes(x=weeks, y=d$'2000', color="2000")) +
        geom_line(aes(x=weeks, y=d$'2001', color="2001")) +
        geom_line(aes(x=weeks, y=d$'2002', color="2002")) +
        geom_line(aes(x=shortWeeks, y=d$'2003', color="2003")) +
        geom_point(aes(x=weeks, y=d$'1995', color="1995")) +
        geom_point(aes(x=weeks, y=d$'1996', color="1996")) +
        geom_point(aes(x=weeks, y=d$'1997', color="1997")) +
```

```
        geom_point(aes(x=weeks, y=d$'1998', color="1998")) +
        geom_point(aes(x=weeks, y=d$'1999', color="1999")) +
        geom_point(aes(x=weeks, y=d$'2000', color="2000")) +
        geom_point(aes(x=weeks, y=d$'2001', color="2001")) +
        geom_point(aes(x=weeks, y=d$'2002', color="2002")) +
        geom_point(aes(x=shortWeeks, y=d$'2003', color="2003")) +
        ggtitle(title) + ylab(title)
    return(p)
}
mortPlot <- plotData(mortData, "Mortality")
infPlot  <- plotData(infData, "Influenza")
tempPlot <- plotData(tempData, "Temperature Deficit")
mortPlot
infPlot
tempPlot

# Training GAM
model <- gam (
            Mortality ~ Year +
            s(Week, k = length(unique(data$Week))),
            data=data,
            method = "GCV.Cp"
        )
summary(model)
modelMean <- mean(model$y)
modelVar <- var(model$y)
print("Train predictions mean:")
modelMean
print("Train predictions variance:")
modelVar
plot(model, main="Smooth Approximation of Mortality")

# Predictions
predictions <- predict(model, data)
ggplot(data) +
    geom_point(aes(x=Time, y=Mortality, color="Real")) +
    geom_line(aes(x=Time, y=predictions, color="Predicted"), size=1) +
    ggtitle("Real and Predicted Mortality")

# Plot GAM predictions per year
plotAll <- function(d, p, title) {
    shortWeeks <- 1:length(d$'2003')
    a <- ggplot() +
        geom_point(aes(x=weeks, y=d$'1995')) +
        geom_point(aes(x=weeks, y=d$'1996')) +
        geom_point(aes(x=weeks, y=d$'1997')) +
        geom_point(aes(x=weeks, y=d$'1998')) +
        geom_point(aes(x=weeks, y=d$'1999')) +
        geom_point(aes(x=weeks, y=d$'2000')) +
        geom_point(aes(x=weeks, y=d$'2001')) +
        geom_point(aes(x=weeks, y=d$'2002')) +
        geom_point(aes(x=shortWeeks, y=d$'2003')) +
        geom_line(aes(x=weeks, y=p$'1995', color="1995")) +
```

```
        geom_line(aes(x=weeks, y=p$'1996', color="1996")) +
        geom_line(aes(x=weeks, y=p$'1997', color="1997")) +
        geom_line(aes(x=weeks, y=p$'1998', color="1998")) +
        geom_line(aes(x=weeks, y=p$'1999', color="1999")) +
        geom_line(aes(x=weeks, y=p$'2000', color="2000")) +
        geom_line(aes(x=weeks, y=p$'2001', color="2001")) +
        geom_line(aes(x=weeks, y=p$'2002', color="2002")) +
        geom_line(aes(x=shortWeeks, y=p$'2003', color="2003")) +
        ggtitle(title)
    return(a)
}

preds <- list()
for (i in 1:length(years)) {
    year <- years[i]
    d <- data[which(data$Year == year),]
    preds[[i]] <- predict(model, d)
}
names(preds) <- years
p <- plotAll(mortData, preds, "Mortality Overall Real and Predictions")
p <- p + ylab("Mortality")
p

# significant terms.
orderedCoefficients <- model$coefficients[order(model$coefficients, decreasing = TRUE)]
print("The 10 most important coefficients:")
orderedCoefficients[1:10]


# Penalty factor analysis
penalties <- c(1e-6, 1e-3, 1, 1e3, 1e6)
predictions <- list()
estDegFreedom <- vector(length = length(penalties))
for (i in 1:length(penalties)) {
    model <- gam (  Mortality ~ Year +
                    s(Week, k = length(unique(data$Week))),
                    data=data,
                    method = "GCV.Cp",
                    sp = penalties[i]
                )
    predictions[[i]] <- predict(model, data)
    estDegFreedom[i] <- summary(model)$edf
}
df <- data.frame(
    time = data$Time,
    real = data$Mortality,
    sp_1u = predictions[[1]],
    sp_1m = predictions[[2]],
    sp_1  = predictions[[3]],
    sp_1k = predictions[[4]],
    sp_1M = predictions[[5]]
)
```

```r
ggplot(df) +
    geom_point(aes(x=time, y=real), color="black") +
    geom_line(aes(x=time, y=sp_1u,  color="sp = 0.000001"), size=1) +
    geom_line(aes(x=time, y=sp_1m,  color="sp = 0.001"), size=1) +
    geom_line(aes(x=time, y=sp_1 ,  color="sp = 1" ), size=1) +
    geom_line(aes(x=time, y=sp_1k,  color="sp = 1000"), size=1) +
    geom_line(aes(x=time, y=sp_1M,  color="sp = 1000000"), size=1) +
    ggtitle("Effects of variations on SP penalization on Spline training") +
    xlab("Time") + ylab("Mortality")


# Relation between penalty factors and degrees of freedom
ggplot() +
    geom_point(aes(x=log10(penalties), y=estDegFreedom)) +
    geom_line(aes(x=log10(penalties), y=estDegFreedom)) +
    ggtitle("Estimated Degrees of Freedom vs SP penalty") +
    ylab("Estimated Degrees of Freedom")


# Comparing model residuals against influenza cases
model <- gam (
                Mortality ~ Year +
                s(Week, k = length(unique(data$Week))),
                data=data,
                method = "GCV.Cp"
              )
ggplot(data) +
    geom_point(aes(x=Time, y=Influenza, color="Influenza")) +
    geom_line(aes(x=Time, y=model$residuals, color="Residuals")) +
    ggtitle("")

# Correlation measurement
corr <- cor(model$residuals, data$Influenza)
print(corr)

# GAM 2 training
model <- gam( formula = Mortality ~ s(Year, k = length(unique(data$Year))) +
                                    s(Week, k = length(unique(data$Week))) +
                                s(Influenza, k=length(unique(data$Influenza))),
              data = data,
              method = "GCV.Cp"
            )
plot(model)

# GAM 2 predictions
predictions <- predict(model, data)
ggplot() +
    geom_point(aes(x=data$Time, y=data$Mortality, color="Real")) +
    geom_line(aes(x=data$Time, y=predictions, color="Predictions")) +
    ggtitle("Second GAM predictions") + ylab("Mortality")
```

Appendix C : Code for Assignment 2

```
################################################################################
##                                 Assignment 2
################################################################################
dataPath <- "data/data.csv"
data <- read.csv2(dataPath)
## Splitting data
splitData <- function(data, trainRate) {
    n <- dim(data)[1]
    idxs <- sample(1:n, floor(trainRate*n))
    train <- data[idxs,]
    test <- data[-idxs,]
    return (list(train = train, test = test))
}

split <- splitData(data, .7)
train <- split$train
test  <- split$test
# Preprocessing
y <- train[[ncol(train)]]
x <- t(train[,-ncol(train)])
mydata <- list(
    x = x,
    y = as.factor(y),
    geneid = as.character(1:nrow(x)),
    genenames = rownames(x)
)

# Training and cross-validating threshold
model <- pamr.train(mydata)
cvmodel <- pamr.cv(model, mydata)
pamr.plotcv(cvmodel)
minError <- min(cvmodel$error)
bestThreshold <- cvmodel$threshold[which.min(cvmodel$error)]

cat("The minimum error is ", minError,
      "and it is obtained for threshold =", bestThreshold)
# best model
bestThreshold <- 1.29
bestModel <- pamr.train(mydata, threshold = bestThreshold)
pamr.plotcen(bestModel, mydata, threshold = bestThreshold)
selectedGenes <- pamr.listgenes(bestModel, mydata,
                                threshold=bestThreshold,
                                genenames = TRUE)
bestGenes <- selectedGenes[1:10,]
cat("There were selected,",nrow(selectedGenes), "features\n")
print("The best 10 selected features are:")
print(bestGenes)
# util function
get_performance <- function(targets, predictions, text) {
    cat("Classification Performance :", text, "\n")
    t <- table(targets, predictions)
    print("Confusion Matrix")
```

```
    print(t)
    tn <- t[1,1]
    tp <- t[2,2]
    fp <- t[1,2]
    fn <- t[2,1]
    total <- sum(t)
    tpr <- tp/(tp+fp) * 100
    tnr <- tn/(tn+fn) * 100
    fpr <- fp/(tp+fp) * 100
    fnr <- fn/(tn+fn) * 100

    cat("Rates details:\n")
    cat(" TPR =", tpr, "% -")
    cat(" TNR =", tnr, "% -")
    cat(" FPR =", fpr, "% -")
    cat(" FNR =", fnr, "%")
    cat("\n Misclassification Rate = ", (fp+fn)/total * 100, "%\n")
}
yTest <- test[[ncol(test)]]
xTest <- t(test[,-ncol(test)])
predictions <- pamr.predict(bestModel, newx = xTest, type = "class",
                            threshold = bestThreshold)
get_performance(yTest, predictions, "Shrunken centroid and shit")

# Elastic-net
cvElastNet <- cv.glmnet(x=t(x), y=y, alpha=.5, type.measure = "mse")
plot(cvElastNet)
optLamdba <- cvElastNet$lambda.min

elasticnetModel <- glmnet(x = t(x), y = y, family="binomial",
                          alpha=.5, lambda = optLamdba)
predictions <- predict(elasticnetModel, newx = t(xTest), type="class")
get_performance(yTest, predictions, "ElasticNet")

coeffs <- coef(elasticnetModel)
nonzeroCoeffs <- coeffs[which(coeffs != 0)]
selectedCoeffs <- length(nonzeroCoeffs)
cat("Elasticnet model has ", selectedCoeffs, " nonzero coefficients\n")

# SVM
svmModel <- ksvm(Conference ~ . , data=train, type="C-svc", kernel="vanilladot")
svmPredictions <- predict(svmModel, test)
get_performance(yTest, svmPredictions, "SVM - Testing performance")

y <- as.factor(data[,ncol(data)])
data <- as.matrix(data[,-ncol(data)])
pvals <- as.numeric(vector(length = ncol(data)))
df <- data.frame(
    word = colnames(data),
    pvals <- pvals
)
BH <- as.numeric(vector(length =ncol(data)))
```

```
FDR <- 0.01
CL  <- 0.95

for(i in 1:length(pvals)) {
    test <- t.test(data[,i] ~ y,
                       alternative = "two.sided",
                       conf.level = CL )
    df[i,2] <- test$p.value
    BH[i] <- (FDR * i / length(pvals))
}

# order increasingly the pvalues
df <- df[order(df$pvals, decreasing = FALSE),]
df <- cbind(df, BH)
L <- max(which(df[,2] < df[,3]))

ggplot() +
    geom_point(aes(x=1:nrow(df), y=df[,2], color="p-values")) +
    geom_line(aes(x=1:nrow(df), y=df[,3], color="BH")) +
    geom_vline(xintercept = L)
cat("Rejected Features =", L, "\n",
    "Rejected Hypothesis Features =" )
for(i in 1:L) {
    cat("\t(", i, ")", as.character(df[i,1]), "\n")
}
```