732A99 chetabook

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Contents

Simple Tasks

Library

```
library("ggplot2") # plots
library("tree") # decision tree
library("caret") # summary and confusion table
library("kknn") # kknn
library("readxl") # reading excel
library("MASS") # Step AIC
library("jtools") # summ function
library("dplyr") # pipelining
library("glmnet") # lasso and ridge
library("mgcv") # spline
library("kernlab") # SVM
library("mboost") # ensemble ADA boost
library("randomForest") # randomforest
library("pamr") # Nearest shrunken
library("boot") # bootstrap
library("fastICA") # fastICA
library("MASS") # LDA
library("neuralnet") # Neural Network
library("e1071") # Naive Bayes

# colours (colour blind friendly)
cbPalette <- c("#999999", "#E69F00", "#56B4E9", "#009E73", "#F0E442", "#0072B2",
               "#D55E00", "#CC79A7")
```

Reading Excel

```
data <- readxl::read_excel("spambase.xlsx", sheet= "spambase_data")
data$Spam <- as.factor(data$Spam)
```

Spliting the Datasets

Divide into train/test

```
data <- readxl::read_excel("spambase.xlsx", sheet= "spambase_data")
data$Spam <- as.factor(data$Spam)
```

```r
# 50-50 split
n=nrow(data)
set.seed(12345)
id=sample(1:n, floor(n*0.5))
train=data[id,]
test=data[-id,]
```

Train/test/validation

```r
data <- readxl::read_excel("spambase.xlsx", sheet= "spambase_data")
data$Spam <- as.factor(data$Spam)
# 50-25-25 split
n=nrow(data)
set.seed(12345)
id=sample(1:n, floor(n*0.5))
train=data[id,]

id1=setdiff(1:n, id)
set.seed(12345)
id2=sample(id1, floor(n*0.25))
valid=data[id2,]

id3=setdiff(id1,id2)
test=data[id3,]
```

Custom code for Cross-Validation

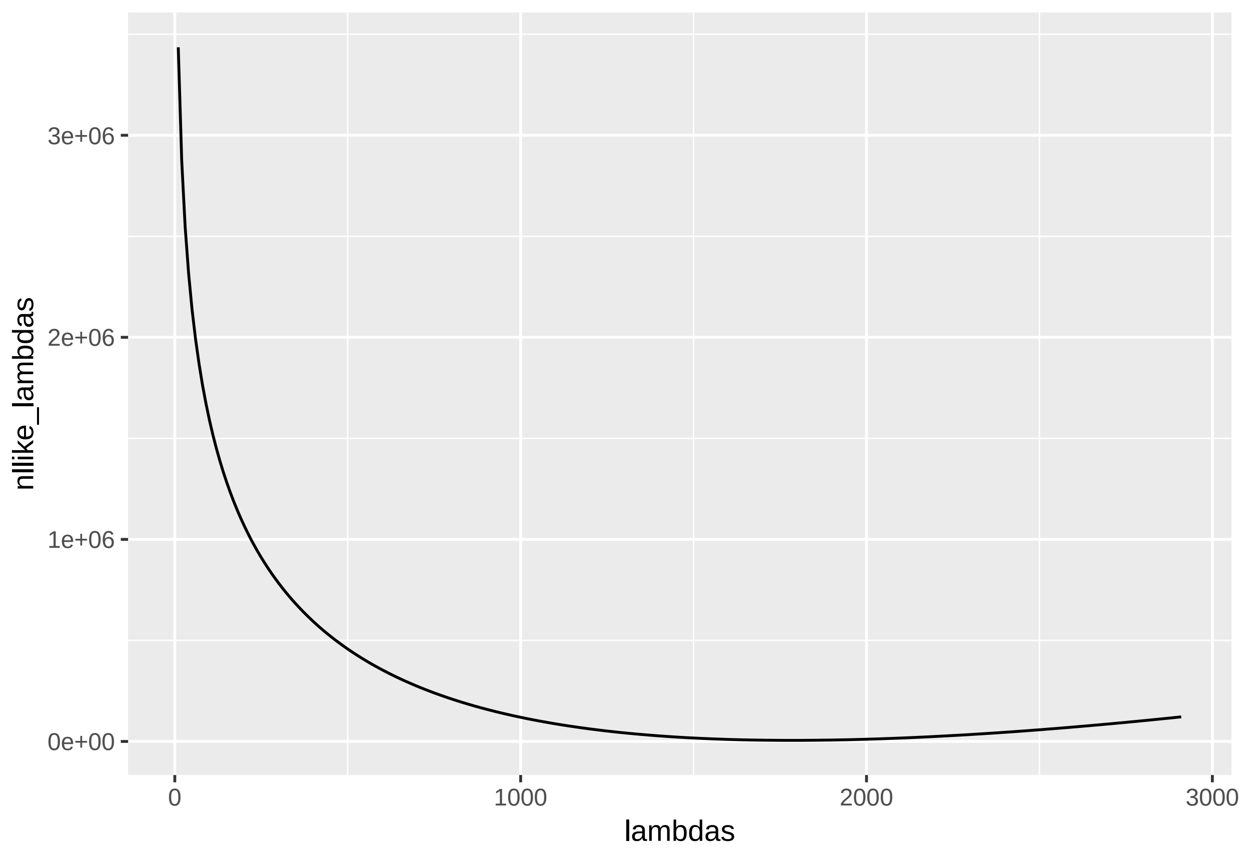
```r
#Randomly shuffle the data
new_data <- data[sample(nrow(data)),]

#Create N equally size folds
new_data$folds <- sample(rep(1:10, each = nrow(new_data)/10))

result <- NULL
#Perform N fold cross validation
for(i in 1:length(unique(new_data$folds))){
  testData <- new_data[new_data$folds != i,]
  trainData <- new_data[new_data$folds == i,]

  #Use the test and train data partitions however you desire, run model code here

  best_model <- glm(formula = Spam ~., family = binomial, data = trainData)
  predicted_value <- predict(best_model, testData, type = "response")
  pred_class <- ifelse(predicted_value > 0.50, 1, 0)
  temp <- 1 - (sum(ifelse(pred_class == testData$Spam,1,0))/nrow(testData))
  temp <- cbind(temp, i)
  colnames(temp) <- c("test_error", "fold")
  result <- rbind(result, temp)
  }
```

Misclassification error calculation

```
missclass=function(X,X1){
  n=length(X)
  return(1-sum(diag(table(X,X1)))/n)
}

#missclass(data2$class, predict(m3, type="class")$class)
```

Assume that mortality y is Poisson distributed, where Y!=1*2*..n . Write an R code computing the minus-loglikelihood of Mortality values for a given lambda. Compute the minus log-likelihood values for lambda=10,110,210,. . . ,2910 and produce a plot showing the dependence of the minus log-likelihood on the value of lambda. Define the optimal value of lambda by means of visual inspection

```
# Loading the data set.
temp_data = read.csv("Influenza.csv")

# Poisson probability function.
prob_y = function(y, lambda){
py = -lambda + (y * log(lambda)) - sum(log(1:y))
return(py)
}

# Negative log likelihood.
neg_llike = function(Y, lambda){
llike = 0
for (y in Y){
llike = llike + prob_y(y, lambda)
}
return(- llike)
}

# Plotting the lambda grids.
lambdas = seq(10, 2910, 10)
nllike_lambdas = c()

for (lambda in lambdas){
nllike_lambdas = c(nllike_lambdas, neg_llike(temp_data$Mortality, lambda))
}
# Plotting the stuff.
ggplot() +
geom_line(aes(x=lambdas, y=nllike_lambdas))
```



```r
# Selecting the lambda that maximizes the
# loglikelihood or that minimizes the negative
# loglikelihood.
min_id = which.min(nllike_lambdas)
best_lambda = lambdas[min_id]
print("The lambda that maximizes the loglikelihood is:")
```

```
## [1] "The lambda that maximizes the loglikelihood is:"
```

```r
## [1] "The lambda that maximizes the loglikelihood is:"
print(best_lambda)
```

```
## [1] 1780
```

Backpropogation Neural Network - Implement the backpropagation algorithm for fitting the parameters of a NN for regression. The NN has one input unit, 10 hidden units, and one output unit. Use the tanh activation function. Recall that you have an example on Bishop's book as well as on the course slides. Feel free to use stochastic or batch gradient descent. Please use only basic R functions in your solution, e.g. sum, tanh.

```r
set.seed(1234567890)
Var = runif(50,0,10)
trva = data.frame(Var, Sin = sin(Var))
tr = trva[1:25,] # training data
```

```r
va = trva[26:50,] # validation data

w_j = runif(10, -1, 1)
b_j = runif(10, -1, 1)
w_k = runif(10, -1, 1)
b_k = runif(1, -1, 1)

l_rate = 1/nrow(tr)^2
n_ite = 5000
error = rep(0, n_ite)
error_va = rep(0, n_ite)

for(i in 1:n_ite) {
  for(n in 1:nrow(tr)) {
    z_j = tanh(w_j * tr[n,]$Var + b_j)
    y_k = sum(w_k * z_j) + b_k

    error[i] = error[i] + (y_k + tr[n,]$Sin)^2
  }

  for(n in 1:nrow(va)) {
    z_j = tanh(w_j * va[n,]$Var + b_j)
    y_k = sum(w_k * z_j) + b_k

    error_va[i] = error_va[i] + (y_k + va[n,]$Sin)^2
  }

  cat("i: ", i , ", error: ", error[i]/2, ", error_va: ", error_va[i]/2, "\n")
  flush.console()

  for(n in 1:nrow(tr)) {
    z_j = tanh(w_j * tr[n,]$Var + b_j)
    y_k = sum(w_k * z_j) + b_k

    d_k = y_k - tr[n,]$Sin
    d_j = (1 - z_j^2) * w_k * d_k
    partial_w_k = d_k * z_j
    partial_b_k = d_k
    partial_w_j = d_j * tr[n,]$Var
    partial_b_j = d_j

    w_k = w_k - l_rate * partial_w_k
    b_k = b_k - l_rate * partial_b_k
    w_j = w_j - l_rate * partial_w_j
    b_j = b_j - l_rate * partial_b_j

  }
}

w_j
b_j
w_k
b_k
```

```r
plot(error/2, ylim = c(0, 5))
points(error_va/2, col = "red")

# prediction on training data

pred = matrix(nrow = nrow(tr), ncol = 2)

for(n in 1:nrow(tr)) {
  z_j = tanh(w_j * tr[n,]$Var + b_j)
  y_k = sum(w_k * z_j) + b_k
  pred[n,] = c(tr[n,]$Var, y_k)
}

plot(pred)
points(tr, col = "red")

# prediction on validation data

pred = matrix(nrow = nrow(va), ncol = 2)

for(n in 1:nrow(va)) {
  z_j = tanh(w_j * va[n,]$Var + b_j)
  y_k = sum(w_k * z_j) + b_k
  pred[n,] = c(va[n,]$Var, y_k)
}

plot(pred)
points(va, col = "red")
```

Regression

Logistics Regression with Decision Boundary

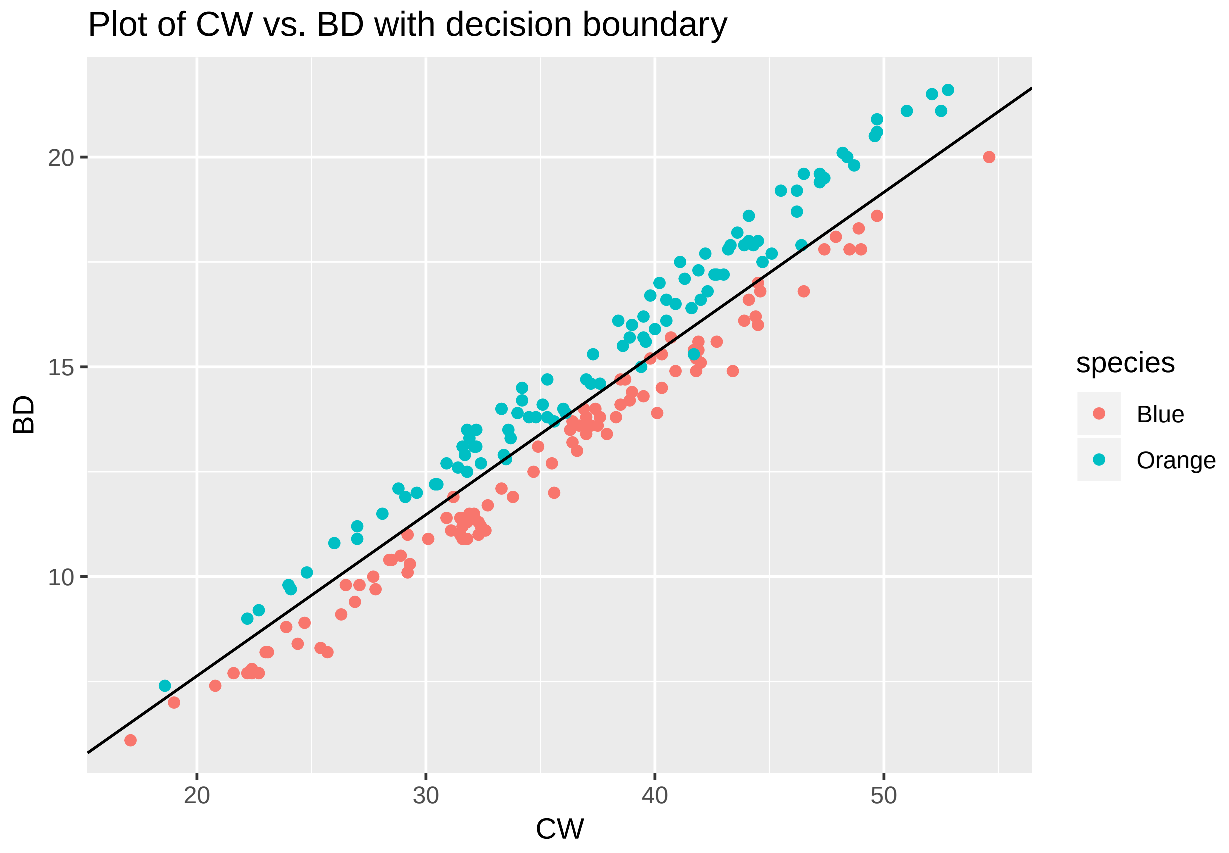
```r
crab_data <- read.csv("australian-crabs.csv")

logistic_model <- glm(formula = species ~ CW + BD, family = binomial, data = crab_data)
summary(logistic_model)
```

```
##
## Call:
## glm(formula = species ~ CW + BD, family = binomial, data = crab_data)
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -1.6442  -0.0459  -0.0001   0.0231   3.5630
##
## Coefficients:
##             Estimate Std. Error z value Pr(>|z|)
## (Intercept)   0.4848     2.8712   0.169    0.866
## CW           -3.6248     0.8229  -4.405 1.06e-05 ***
## BD            9.4328     2.1290   4.431 9.40e-06 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 277.259  on 199  degrees of freedom
## Residual deviance:  31.429  on 197  degrees of freedom
## AIC: 37.429
##
## Number of Fisher Scoring iterations: 9
```

```
crab_data$predicted_species_logisitic_prob <- predict(logistic_model,
                                                      newdata = crab_data, type = "response")

crab_data$predicted_species_logisitic <- ifelse(crab_data$predicted_species_logisitic_prob > 0.50,
                                                "Orange", "Blue")

conf_logistics <- table(crab_data$species, crab_data$predicted_species_logisitic)
names(dimnames(conf_logistics)) <- c("Actual", "Predicted")
caret::confusionMatrix(conf_logistics)
```

```
## Confusion Matrix and Statistics
##
##         Predicted
## Actual   Blue Orange
##   Blue     99      1
##   Orange    3     97
##
##                Accuracy : 0.98
##                  95% CI : (0.9496, 0.9945)
##     No Information Rate : 0.51
##     P-Value [Acc > NIR] : <2e-16
##
##                   Kappa : 0.96
##
##  Mcnemar's Test P-Value : 0.6171
##
##             Sensitivity : 0.9706
##             Specificity : 0.9898
##          Pos Pred Value : 0.9900
##          Neg Pred Value : 0.9700
##              Prevalence : 0.5100
##          Detection Rate : 0.4950
##    Detection Prevalence : 0.5000
##       Balanced Accuracy : 0.9802
##
##        'Positive' Class : Blue
##
```

```
slope <- coef(logistic_model)[2]/(-coef(logistic_model)[3])
intercept <- coef(logistic_model)[1]/(-coef(logistic_model)[3])

ggplot(data=crab_data, aes(x=CW, y=BD, colour = species)) +
  geom_point() +
  geom_abline(intercept = intercept , slope = slope, color = "black") +
  ggtitle("Plot of CW vs. BD with decision boundary")
```



Logistic Regression

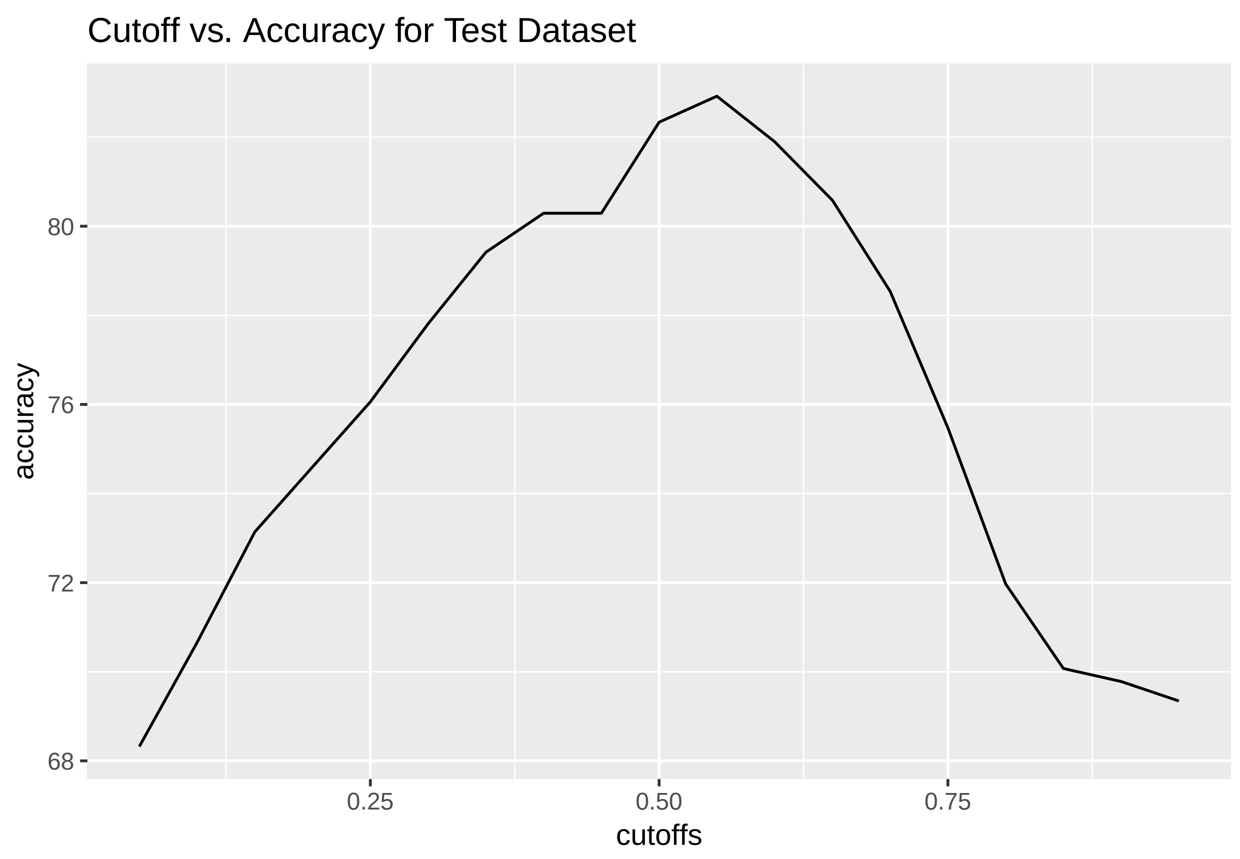
```
best_model <- glm(formula = Spam ~., family = binomial, data = train)
#summary(best_model)

train$prediction_prob <- predict(best_model, newdata = train, type = "response")
train$prediction_class_50 <- ifelse(train$prediction_prob > 0.50, 1, 0)

test$prediction_prob <- predict(best_model, newdata = test, type = "response")
test$prediction_class_50 <- ifelse(test$prediction_prob > 0.50, 1, 0)

conf_train <- table(train$Spam, train$prediction_class_50)
names(dimnames(conf_train)) <- c("Actual Train", "Predicted Train")
caret::confusionMatrix(conf_train)
```

```
## Confusion Matrix and Statistics
##
##             Predicted Train
## Actual Train   0   1
##            0 803 142
##            1  81 344
##
```

```
##                Accuracy : 0.8372
##                  95% CI : (0.8166, 0.8564)
##     No Information Rate : 0.6453
##     P-Value [Acc > NIR] : < 2.2e-16
##
##                   Kappa : 0.6341
##
##  Mcnemar's Test P-Value : 5.872e-05
##
##             Sensitivity : 0.9084
##             Specificity : 0.7078
##          Pos Pred Value : 0.8497
##          Neg Pred Value : 0.8094
##              Prevalence : 0.6453
##          Detection Rate : 0.5861
##    Detection Prevalence : 0.6898
##       Balanced Accuracy : 0.8081
##
##        'Positive' Class : 0
##
```

Choosing the best cutoff for test

```
cutoffs <- seq(from = 0.05, to = 0.95, by = 0.05)
accuracy <- NULL

for (i in seq_along(cutoffs)){
    prediction <- ifelse(test$prediction_prob >= cutoffs[i], 1, 0) #Predicting for cut-off

    accuracy <- c(accuracy,length(which(test$Spam == prediction))/length(prediction)*100)}

cutoff_data <- as.data.frame(cbind(cutoffs, accuracy))

ggplot(data = cutoff_data, aes(x = cutoffs, y = accuracy)) +
  geom_line() +
  ggtitle("Cutoff vs. Accuracy for Test Dataset")
```



KKNN

```
knn_model30 <- train.kknn(Spam ~., data = train, kmax = 30)

test$knn_prediction_class <- predict(knn_model30, test)

conf_test2 <- table(test$Spam, test$knn_prediction_class)
names(dimnames(conf_test2)) <- c("Actual Test", "Predicted Test")
confusionMatrix(conf_test2)
```

```
## Confusion Matrix and Statistics
##
##            Predicted Test
## Actual Test   0   1
##           0 402  74
##           1  66 143
##
##                Accuracy : 0.7956
##                  95% CI : (0.7634, 0.8252)
##     No Information Rate : 0.6832
##     P-Value [Acc > NIR] : 3.278e-11
##
##                   Kappa : 0.5231
##
##  Mcnemar's Test P-Value : 0.5541
```

```
##
##             Sensitivity : 0.8590
##             Specificity : 0.6590
##          Pos Pred Value : 0.8445
##          Neg Pred Value : 0.6842
##              Prevalence : 0.6832
##          Detection Rate : 0.5869
##    Detection Prevalence : 0.6949
##       Balanced Accuracy : 0.7590
##
##        'Positive' Class : 0
##
```

Step AIC

```r
tecator_data <- readxl::read_excel("tecator.xlsx", sheet = "data")
tecator_data <- tecator_data[,2:NCOL(tecator_data)] # removing sample column


min.model1 = lm(Fat ~ 1, data=tecator_data[,-1])
biggest1 <- formula(lm(Fat ~.,  data=tecator_data[,-1]))

step.model1 <- stepAIC(min.model1, direction ='forward', scope=biggest1, trace = FALSE)
summ(step.model1)
```

Observations	215
Dependent variable	Fat
Type	OLS linear regression

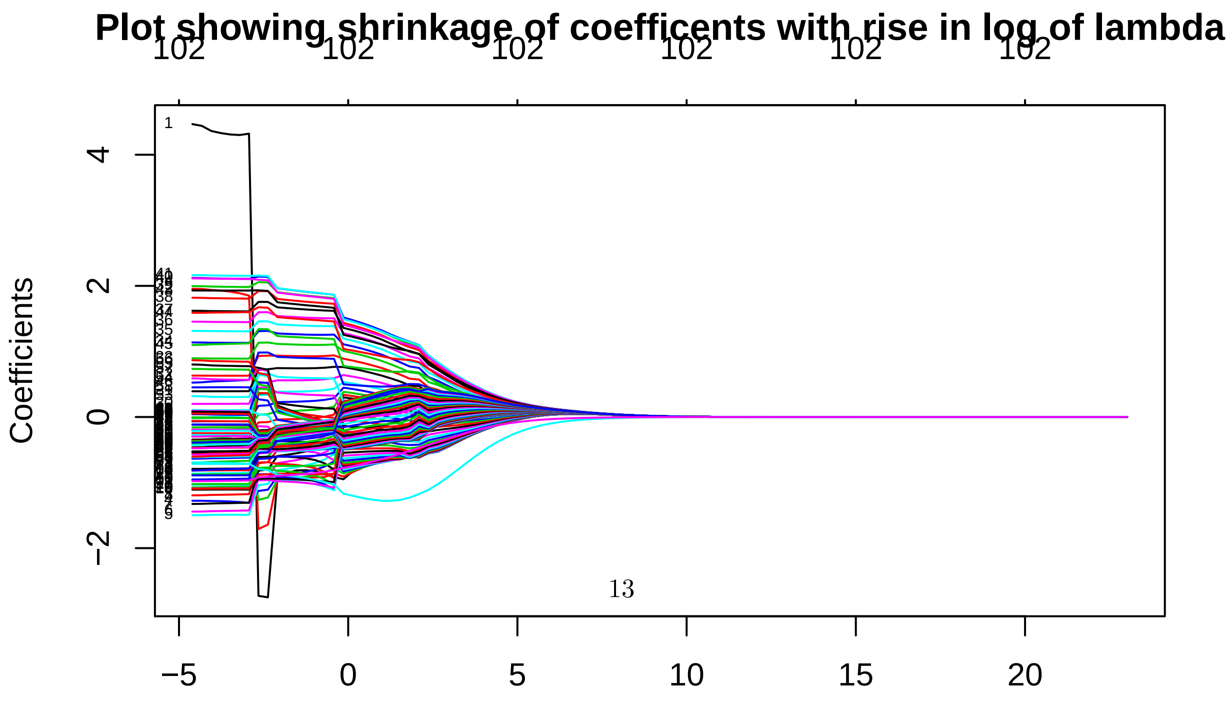
F(29,185)	4775.35
R^2	1.00
Adj. R^2	1.00

Ridge Regression

```r
y <- tecator_data %>% select(Fat) %>% data.matrix()
x <- tecator_data %>% select(-c(Fat)) %>% data.matrix()

lambda <- 10^seq(10, -2, length = 100)

ridge_fit <- glmnet(x, y, alpha = 0, family = "gaussian", lambda = lambda)
plot(ridge_fit, xvar = "lambda", label = TRUE,
     main = "Plot showing shrinkage of coefficents with rise in log of lambda")
```

	Est.	S.E.	t val.	p
(Intercept)	93.46	1.59	58.86	0.00
Moisture	-1.03	0.02	-54.25	0.00
Protein	-0.64	0.06	-10.91	0.00
Channel100	66.56	48.18	1.38	0.17
Channel41	-3268.11	826.92	-3.95	0.00
Channel7	-64.03	20.80	-3.08	0.00
Channel48	-2022.46	254.46	-7.95	0.00
Channel42	4934.22	1124.96	4.39	0.00
Channel50	1239.52	236.09	5.25	0.00
Channel45	4796.22	783.38	6.12	0.00
Channel66	2435.79	1169.85	2.08	0.04
Channel56	2373.00	540.06	4.39	0.00
Channel90	-258.27	247.22	-1.04	0.30
Channel60	-264.27	708.11	-0.37	0.71
Channel70	14.25	327.12	0.04	0.97
Channel67	-2015.92	543.74	-3.71	0.00
Channel59	635.71	996.31	0.64	0.52
Channel65	-941.61	1009.23	-0.93	0.35
Channel58	1054.24	927.95	1.14	0.26
Channel44	-5733.84	1079.19	-5.31	0.00
Channel18	299.80	88.43	3.39	0.00
Channel78	2371.11	361.25	6.56	0.00
Channel84	-428.99	338.35	-1.27	0.21
Channel62	3062.97	769.59	3.98	0.00
Channel53	-804.39	203.44	-3.95	0.00
Channel75	-1461.42	402.26	-3.63	0.00
Channel57	-3266.79	876.71	-3.73	0.00
Channel63	-2844.66	906.40	-3.14	0.00
Channel24	-308.71	97.87	-3.15	0.00
Channel37	401.64	151.76	2.65	0.01

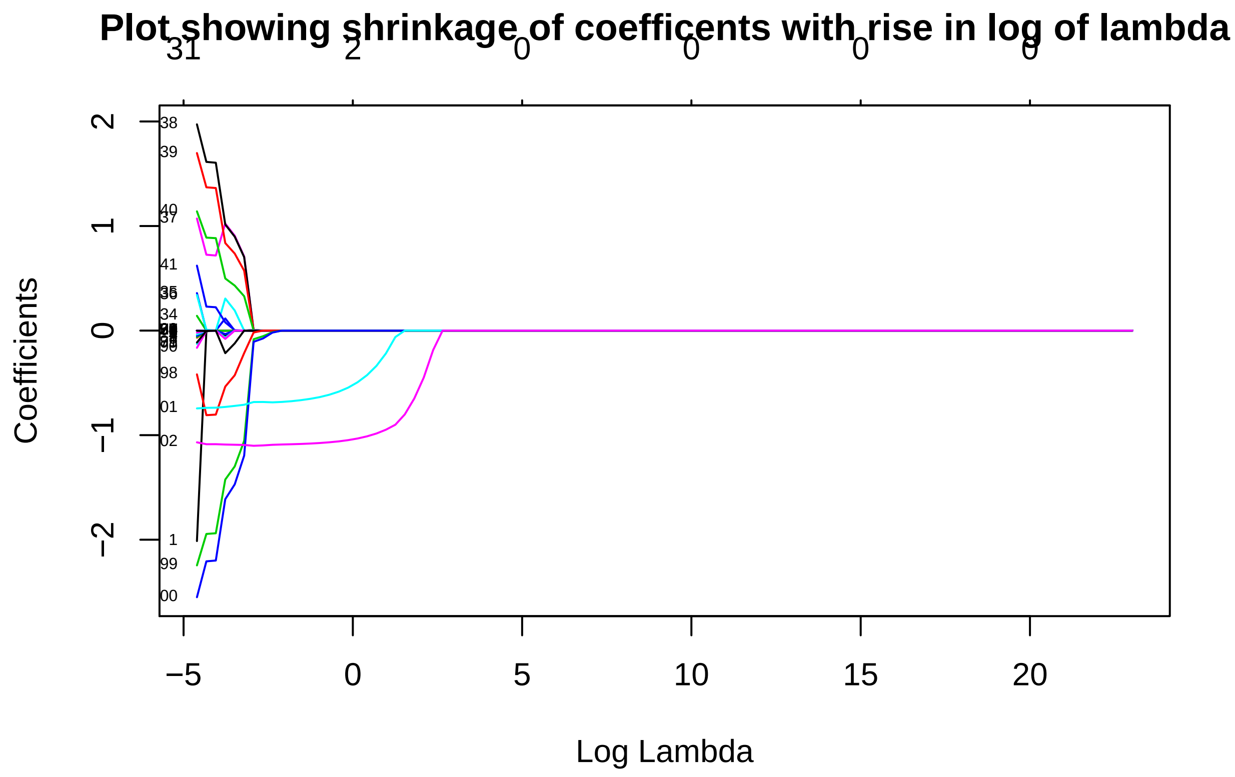
Standard errors: OLS



```
## Change of coefficent with respect to lambda
result <- NULL
for(i in lambda){
temp <- t(coef(ridge_fit, i)) %>% as.matrix()
temp <- cbind(temp, lambda = i)
result <- rbind(temp, result)
}
result <- result %>% as.data.frame() %>% arrange(lambda)
#head(result,10)
```

Lasso Regression

```
lambda <- 10^seq(10, -2, length = 100)

lasso_fit <- glmnet(x, y, alpha = 1, family = "gaussian", lambda = lambda)
plot(lasso_fit, xvar = "lambda", label = TRUE,
     main = "Plot showing shrinkage of coefficents with rise in log of lambda")
```



Lasso Regression using Cross Validation

```
#find the best lambda from our list via cross-validation
```

```r
data <- read.csv("Influenza.csv")
data_scaled <- data %>% select(-c("Mortality")) %>%
  scale() %>% cbind(Mortality = data$Mortality) %>% as.data.frame()

### 50-50 split
n=nrow(data_scaled)
set.seed(12345)
id=sample(1:n, floor(n*0.5))
train=data_scaled[id,]
test=data_scaled[-id,]


lambda <- 10^seq(10, -2, length = 100)

X <- train %>% select(-c("Mortality")) %>% as.matrix()
Y <- train %>% select(c("Mortality")) %>% as.matrix()
X_test <- test %>% select(-c("Mortality")) %>% as.matrix()
Y_test <- test %>% select(c("Mortality")) %>% as.vector()


lambda_lasso <- 10^seq(10, -2, length = 100)
lambda_lasso[101] <- 0
lasso_cv <- cv.glmnet(X,Y, alpha=1, lambda = lambda_lasso, type.measure="mse")

#coef(lasso_cv, lambda = lasso_cv$lambda.min)

## lambda.min and lambda.se the difference is as follows
## lambda.min gives the lambda value for absolute min error
## while lambda.se gives lambda value for a very regularized model with error within one std error of l

min_lambda <- lasso_cv$lambda.min

## Retaining the best model and predicting

### best model
best_lasso <- glmnet(X, Y, alpha = 1, family = "poisson", lambda = min_lambda)


### printing the mse
Y_test$predict_y <- predict(best_lasso, newx = X_test, type = "response")
Y_test$MSE <- (Y_test$predict_y - Y_test$Mortality)^2

### alpha value
cat("The beta from the model are:")
```

```
## The beta from the model are:
```

```r
best_lasso$beta
```

```
## 8 x 1 sparse Matrix of class "dgCMatrix"
##                                 s0
## Year                    .
## Week                 -0.007212981
## Influenza             0.015746431
## Temperature.deficit   0.018030934
## Influenza_lag1       0.004854973
## Temp_lag1            0.007778392
## Influenza_lag2       0.022747261
## Temp_lag2            0.007465742
```

```
# or coef(best_lasso)

cat("The alpha value is: ", best_lasso$a0, "while the exp value of alpha is: ", exp(best_lasso$a0))
```

```
## The alpha value is:  7.481289 while the exp value of alpha is:  1774.526
```

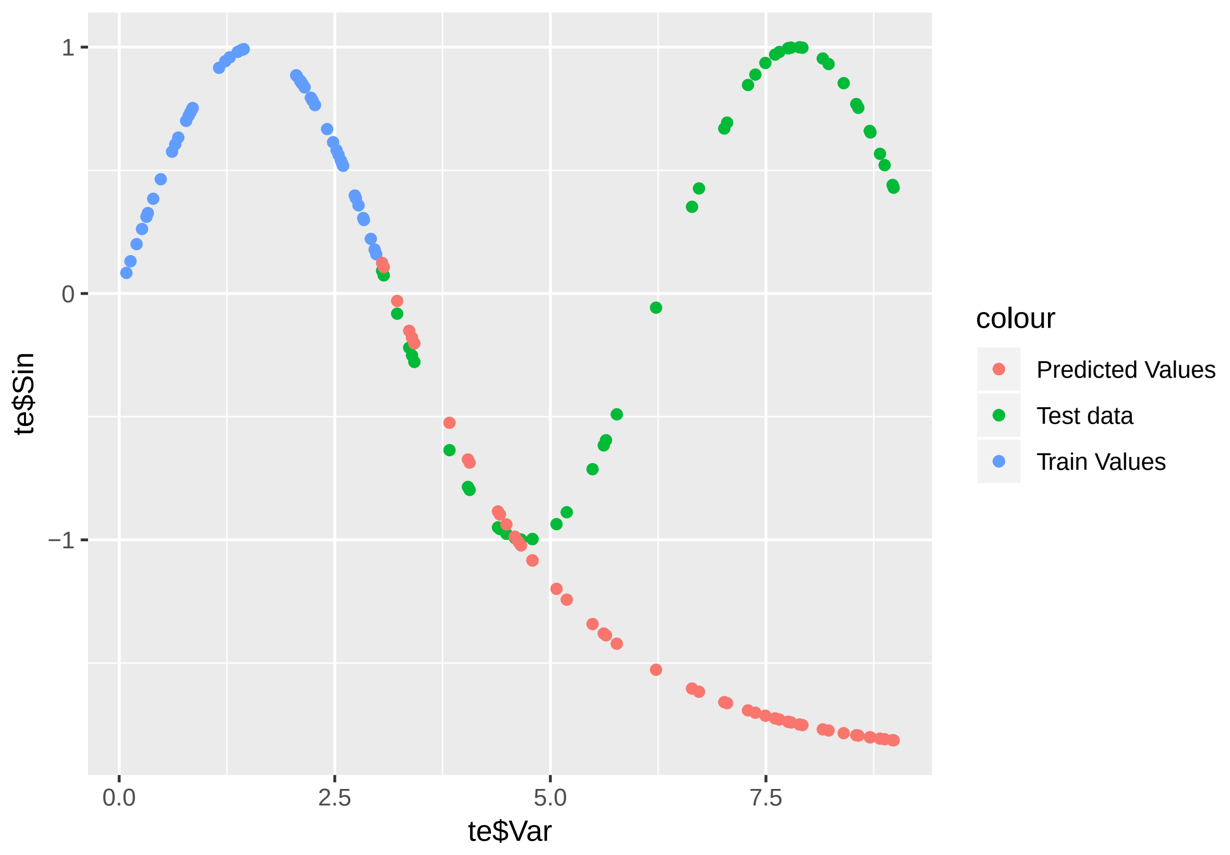
```
cat("The mean squared error is:", mean(Y_test$MSE))
```

```
## The mean squared error is: 11646.36
```

```
### Change of coefficent with respect to lambda
result_lasso <- NULL
for(i in 1:length(lambda_lasso)){
temp <- lasso_cv$cvm[i] %>% as.matrix()
temp <- cbind(CVM_error = temp, lambda = lasso_cv$lambda[i])
result_lasso <- rbind(temp, result_lasso)
}

#head(result_lasso,10)
```

Neural Network

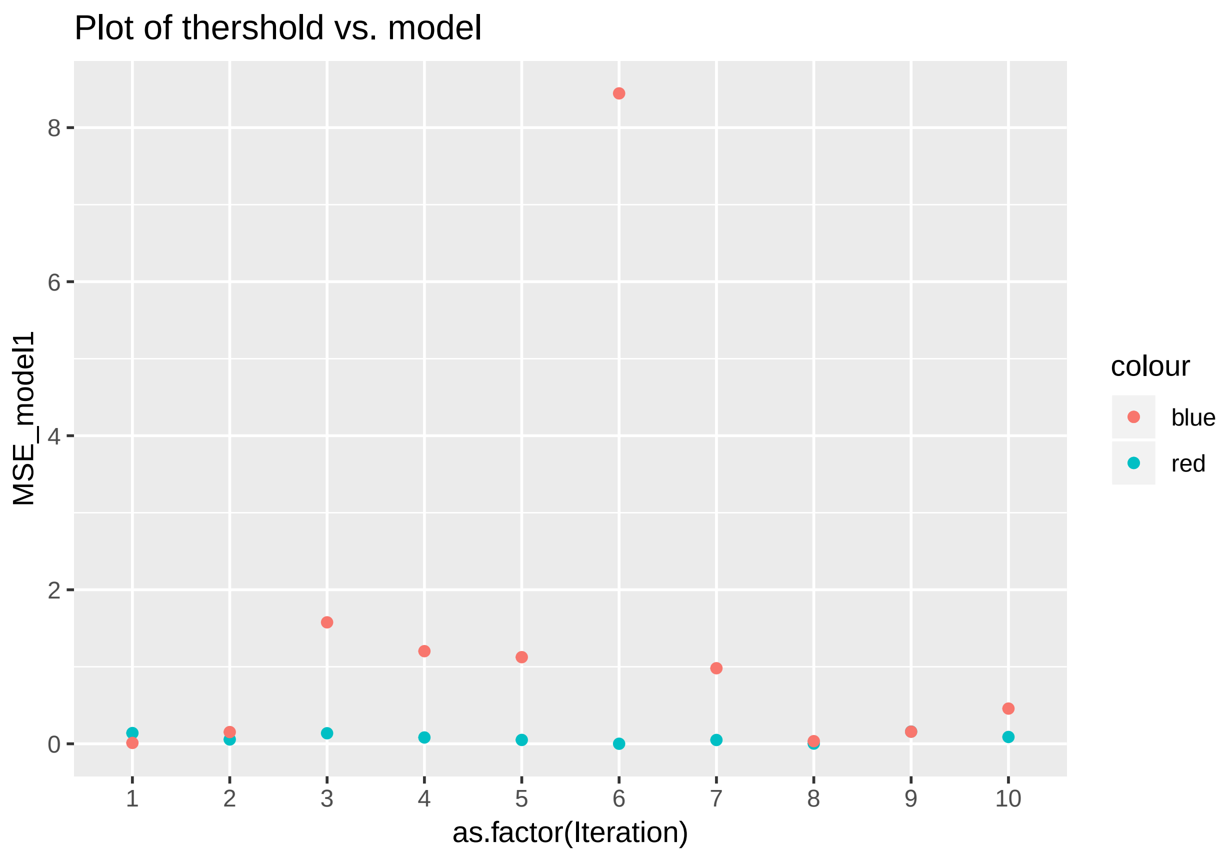
```
# Doing as told by the exam instructions.
set.seed(1234567890)

Var = runif(50, 0, 3)
tr = data.frame(Var, Sin=sin(Var))
Var = runif(50, 3, 9)
te = data.frame(Var, Sin=sin(Var))

# Random initialization of the weights in the interval [-1, 1].
winit = runif(10, -1, 1)

# Training the neural network on the train set.
nn = neuralnet(Sin ~ Var, data=tr, hidden=c(3), startweights=winit)

# Getting the predictions, compute is depracted, never use it
yhat_test = predict(object = nn, newdata = te)

# Plotting the plotty mc plot face.
p = ggplot2::ggplot() +
    ggplot2::geom_point(ggplot2::aes(x=te$Var, y=te$Sin, color="Test data")) +
    ggplot2::geom_point(ggplot2::aes(x=tr$Var, y=tr$Sin, color="Train Values")) +
    ggplot2::geom_point(ggplot2::aes(x=te$Var, y=yhat_test, color="Predicted Values"))
print(p)
```



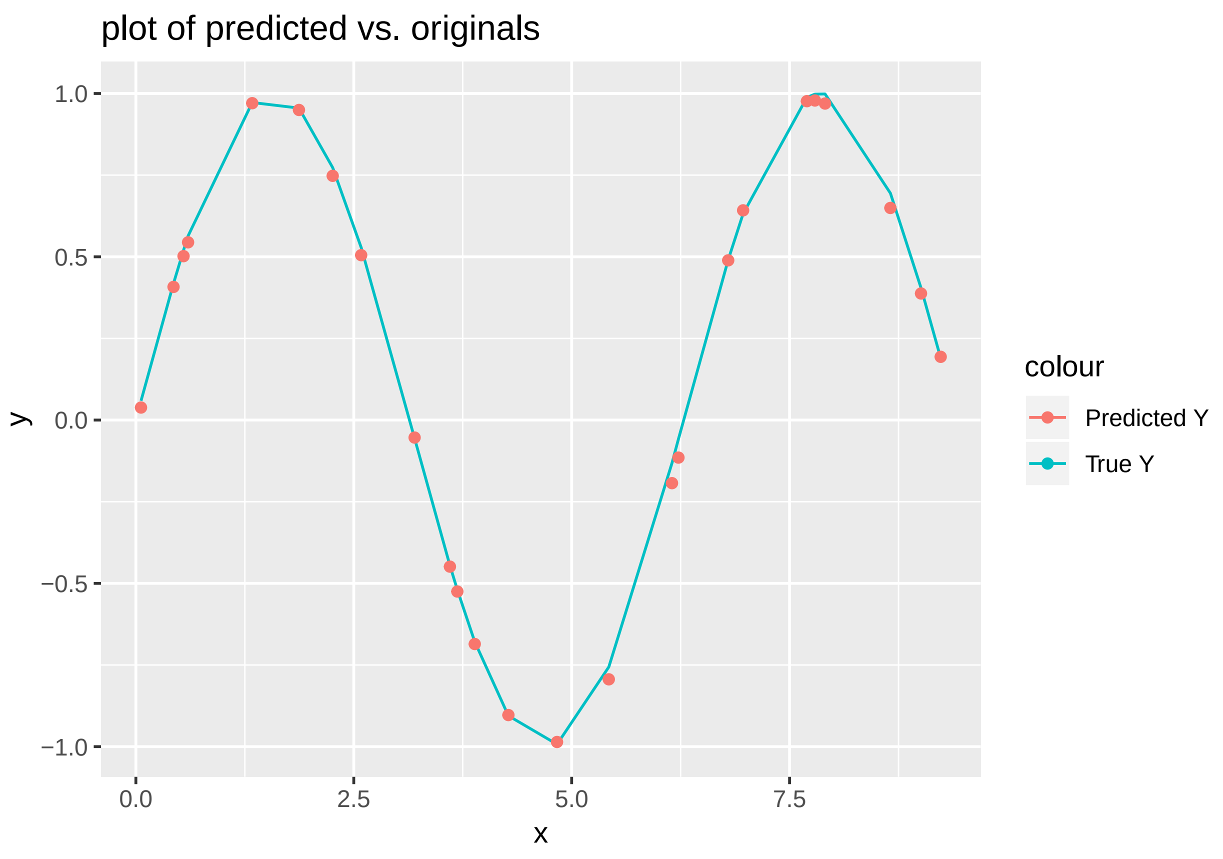
Train a neural network to learn the trigonometric sine function. To do so, sample 50 points uniformly at random in the interval [0, 10]. Apply the sine function to each point. The resulting pairs are the data available to you. Use 25 of the 50 points for training and the rest for validation. The validation set is used for early stop of the gradient descent. Consider threshold values i*0.01 with i = 1,2,. . . ,10. Initialize the weights of the neural network to random values in the interval [???1, 1]. Consider two NN architectures: A single hidden layer of 10 units, and two hidden layers with 3 units each. Choose the most appropriate NN architecture and threshold value. Motivate your choice. Feel free to reuse the code of the corresponding lab.

```r
set.seed(12345)
x <- sample(seq(0,10,0.001),50)
y <- sin(x)
sin_data <- cbind(x,y)
sin_data <- as.data.frame(sin_data)
colnames(sin_data) <- c("x", "y")

train <- sin_data[1:25,]
valid <- sin_data[26:50,]

run_weights = runif(n=10, min=-1, max = 1)

final <- NULL
for(i in 1:10){
```

```
model_1_hidden <- neuralnet(y~x, data=train, hidden=c(10), startweights = run_weights, threshold = i * 
model_2_hidden <- neuralnet(y~x, data=train, hidden=c(3,3), startweights = run_weights, threshold = i *

# predicted_value
predicted_y_model1 <- predict(model_1_hidden, newdata = valid)
predicted_y_model2 <- predict(model_2_hidden, newdata = valid)
mse_model1 <- sum(predicted_y_model1 - valid$y)^2
mse_model2 <- sum(predicted_y_model2 - valid$y)^2
temp <- cbind(mse_model1, mse_model2, i)
final <- rbind(temp, final)
}

colnames(final) <- c("MSE_model1", "MSE_model2", "Iteration")
final <- as.data.frame(final)

ggplot(data=final, aes(x=as.factor(Iteration))) +
  geom_point(aes(y = MSE_model1 ,color="red")) +
  geom_point(aes(y = MSE_model2 ,color="blue")) +
  ggtitle("Plot of thershold vs. model")
```



```
# from the dataset seens, the best model is model1 and thershold is 6 * 0.001

best_model <- neuralnet(y~x, data=train, hidden=c(10), startweights = run_weights, threshold = 6 * 0.00
valid$predicted_y <- predict(best_model, newdata = valid)

ggplot(data=valid) +
  geom_line(aes(x=x, y=y, color="True Y")) +
  geom_point(aes(x=x, y=predicted_y, color="Predicted Y")) +
  ggtitle("plot of predicted vs. originals")
```



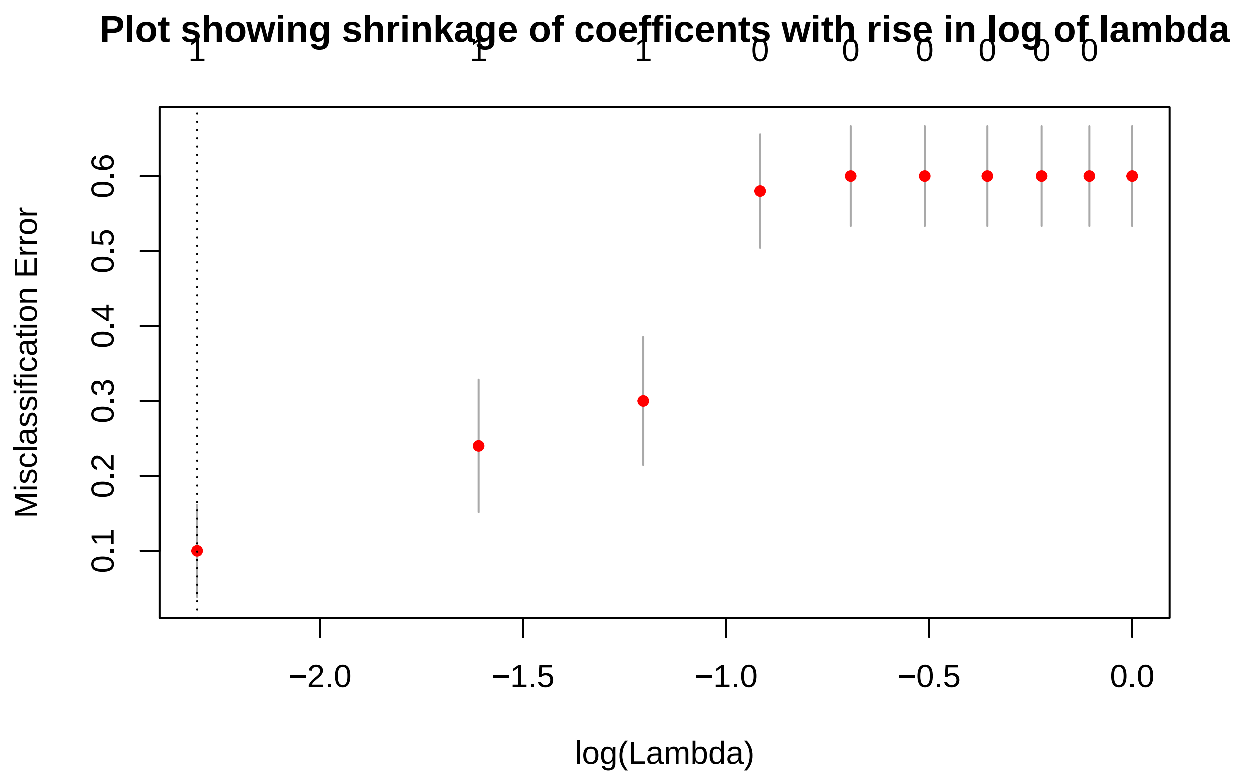
Classification

LASSO

```
n=NROW(iris)
set.seed(12345)
id=sample(1:n, floor(n*1/3))
train=iris[id,]
id1=setdiff(1:n, id)
set.seed(12345)
id2=sample(id1, floor(n*1/3))
valid=iris[id2,]
id3=setdiff(id1,id2)
test=iris[id3,]

y <- train %>% select(Species) %>% data.matrix()
x <- train %>% select(-c(Species)) %>% data.matrix()

y_valid <- valid %>% select(Species) %>% data.matrix()
```

```
x_valid <- valid %>% select(-c(Species)) %>% data.matrix()

lambda <- seq(from=0, to=1, by=0.1)
lasso_fit <- cv.glmnet(x, y, alpha = 1, family = "multinomial", lambda = lambda, type.measure = "class"
plot(lasso_fit, xvar = "lambda", label = TRUE,
main = "Plot showing shrinkage of coefficents with rise in log of lambda")
```

```
## Warning in plot.window(...): "xvar" is not a graphical parameter

## Warning in plot.window(...): "label" is not a graphical parameter

## Warning in plot.xy(xy, type, ...): "xvar" is not a graphical parameter

## Warning in plot.xy(xy, type, ...): "label" is not a graphical parameter

## Warning in axis(side = side, at = at, labels = labels, ...): "xvar" is not
## a graphical parameter

## Warning in axis(side = side, at = at, labels = labels, ...): "label" is not
## a graphical parameter

## Warning in axis(side = side, at = at, labels = labels, ...): "xvar" is not
## a graphical parameter

## Warning in axis(side = side, at = at, labels = labels, ...): "label" is not
## a graphical parameter

## Warning in box(...): "xvar" is not a graphical parameter

## Warning in box(...): "label" is not a graphical parameter

## Warning in title(...): "xvar" is not a graphical parameter

## Warning in title(...): "label" is not a graphical parameter
```



```
min_lambda <- lasso_fit$lambda.min

best_model <- glmnet(x,y,alpha = 1, family = "multinomial", lambda = min_lambda)

predicted <- predict(best_model, newx = x_valid, type=c("class"))
new_predicted <- cbind(predicted, y_valid) %>% as.data.frame()
colnames(new_predicted) <- c("Predicted_class", "Actual_class")

lasso_confusion <- table(new_predicted$Predicted_class, new_predicted$Actual_class)
names(dimnames(lasso_confusion)) <- c("Predicted Validation", "Actual Validation")
caret::confusionMatrix(lasso_confusion)
```

```
## Confusion Matrix and Statistics
##
##                       Actual Validation
## Predicted Validation  1  2  3
##                     1 19  0  0
##                     2  0 16  2
##                     3  0  2 11
##
## Overall Statistics
##
##                Accuracy : 0.92
##                  95% CI : (0.8077, 0.9778)
##     No Information Rate : 0.38
##     P-Value [Acc > NIR] : 1.678e-15
```

```
##
##                   Kappa : 0.8785
##
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: 1 Class: 2 Class: 3
## Sensitivity              1.00   0.8889   0.8462
## Specificity              1.00   0.9375   0.9459
## Pos Pred Value           1.00   0.8889   0.8462
## Neg Pred Value           1.00   0.9375   0.9459
## Prevalence               0.38   0.3600   0.2600
## Detection Rate           0.38   0.3200   0.2200
## Detection Prevalence     0.38   0.3600   0.2600
## Balanced Accuracy        1.00   0.9132   0.8960
```

Naive Bayes, using default threshold

```r
set.seed(12345)
credit_data <- readxl::read_excel("creditscoring.xls", sheet = "credit")
credit_data$good_bad <- as.factor(credit_data$good_bad)

n=NROW(credit_data)
set.seed(12345)
id=sample(1:n, floor(n*0.5))
train=credit_data[id,]

id1=setdiff(1:n, id)
set.seed(12345)
id2=sample(id1, floor(n*0.25))
valid=credit_data[id2,]

id3=setdiff(id1,id2)
test=credit_data[id3,]

#Fitting the Naive Bayes model
credit_naive_model = e1071::naiveBayes(good_bad ~., data=train)

#Prediction on the dataset
predict_naive_train = predict(credit_naive_model, newdata=train, type = "class")
predict_naive_test = predict(credit_naive_model, newdata=test, type = "class")

conf_naive_train <- table(train$good_bad, predict_naive_train)
names(dimnames(conf_naive_train)) <- c("Actual Train", "Predicted Train")
caret::confusionMatrix(conf_naive_train)
```

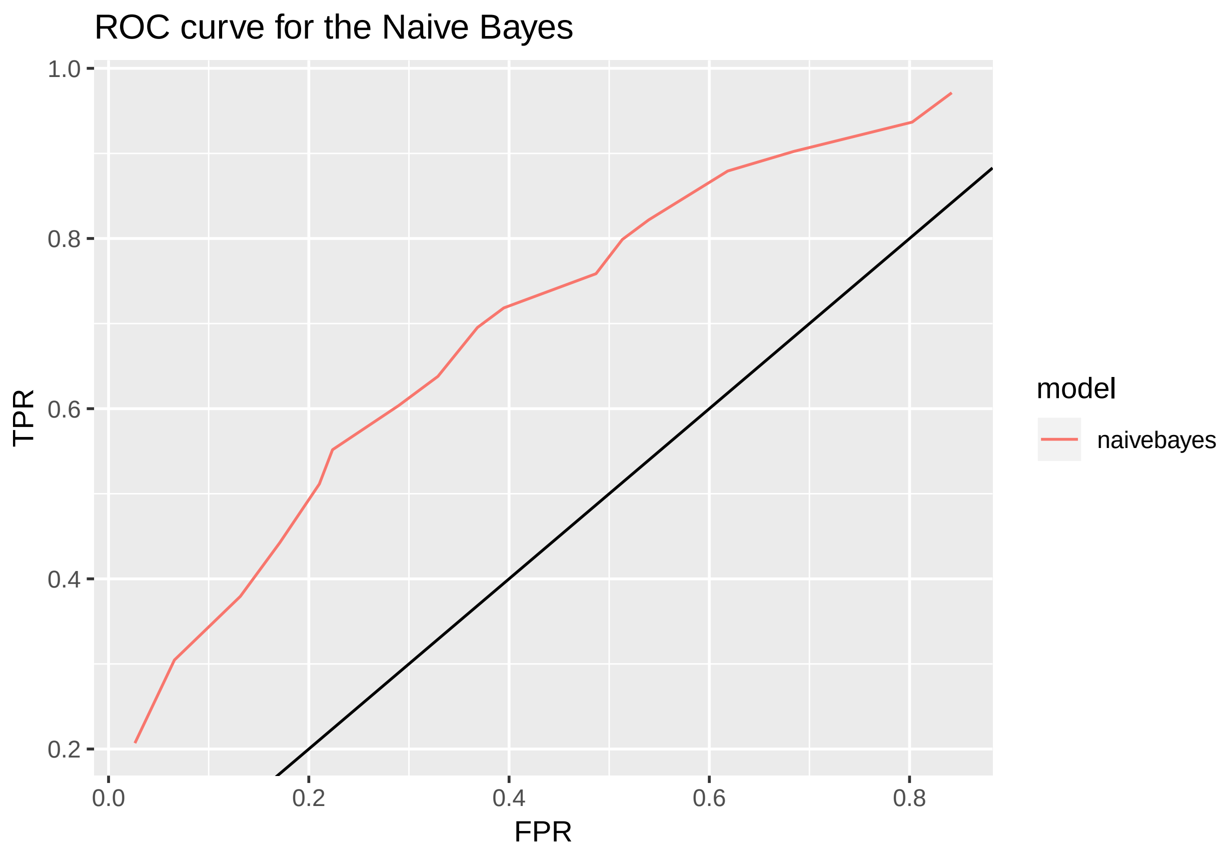
```
## Confusion Matrix and Statistics
##
##             Predicted Train
## Actual Train bad good
##         bad   95   52
##         good  98  255
```

```
##
##                Accuracy : 0.7
##                  95% CI : (0.6577, 0.7399)
##     No Information Rate : 0.614
##     P-Value [Acc > NIR] : 3.655e-05
##
##                   Kappa : 0.3378
##
##  Mcnemar's Test P-Value : 0.0002386
##
##             Sensitivity : 0.4922
##             Specificity : 0.8306
##          Pos Pred Value : 0.6463
##          Neg Pred Value : 0.7224
##              Prevalence : 0.3860
##          Detection Rate : 0.1900
##    Detection Prevalence : 0.2940
##       Balanced Accuracy : 0.6614
##
##        'Positive' Class : bad
##
```

Naive Bayes varying threshold and ROC curve

```
# model
credit_naive_model = e1071::naiveBayes(good_bad ~., data=train)

# predicting class, getting probability
predict_naive_test_prob <- predict(credit_naive_model, newdata=test, type = "raw")

# data mugging
probability_data_naive <- as.data.frame(cbind(predict_naive_test_prob,
                                               as.character(test$good_bad), "naivebayes"))

colnames(probability_data_naive) <- c("prob_bad", "prob_good",
                                          "actual_test_class", "model")

# final dataset
probability_data_naive$prob_good <- as.numeric(as.character(probability_data_naive$prob_good))



naive_list <- NULL
final <- NULL

for(threshold in seq(from = 0.05, to = 0.95, by = 0.05)){
 probability_data_naive$predicted_class <- ifelse(probability_data_naive$prob_good > threshold,
                                                  "good", "bad")

  df2 <- probability_data_naive[,c("model", "actual_test_class", "predicted_class")]
  df2$threshold <- threshold
  df2$match <- ifelse(df2$actual_test_class == df2$predicted_class, 1, 0)
```

```r
  final <- rbind(df2, final)
}

# Creating the FRP and TRP for each model and threshold
final$temp <- 1

final_summary <- final %>%
group_by(model, threshold) %>%
summarise(total_positive = sum(temp[actual_test_class == "good"]),
          total_negative = sum(temp[actual_test_class == "bad"]),
          correct_positive = sum(temp[actual_test_class == "good" & predicted_class == "good"]),
          false_positive = sum(temp[actual_test_class == "bad" & predicted_class == "good"])) %>%
  mutate(TPR = correct_positive/total_positive, FPR = false_positive/total_negative)

ggplot(data = final_summary, aes(x = FPR, y=TPR)) + geom_line(aes(colour = model)) +
  geom_abline(intercept = 0.0, slope = 1) +
  ggtitle("ROC curve for the Naive Bayes")
```



Decision trees (tree lib)

```r
set.seed(12345)

data <- read.csv("crx.csv", header = TRUE)
data$Class <- as.factor(data$Class)
```

```r
# 50-50 split
n=nrow(data)
id=sample(1:n, floor(n*0.8))
train=data[id,]
test=data[-id,]

tree_deviance <- tree::tree(Class~., data=train, split = c("deviance"))
tree_gini <- tree::tree(Class~., data=train, split = c("gini"))

# Visualize the decision tree with rpart.plot
summary(tree_deviance)
```

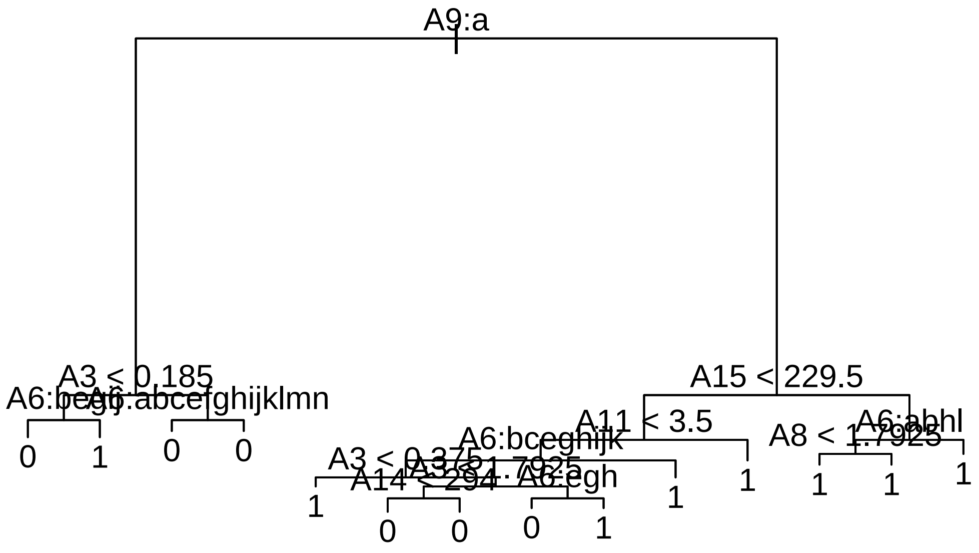
```
##
## Classification tree:
## tree::tree(formula = Class ~ ., data = train, split = c("deviance"))
## Variables actually used in tree construction:
## [1] "A9"  "A3"  "A6"  "A15" "A11" "A14" "A8"
## Number of terminal nodes:  14
## Residual mean deviance:  0.4752 = 255.6 / 538
## Misclassification error rate: 0.09601 = 53 / 552
```

```r
# predicting on the test dataset to get the misclassification rate.
predict_tree_deviance <- predict(tree_deviance, newdata = test, type = "class")
predict_tree_gini <- predict(tree_deviance, newdata = test, type = "class")

conf_tree_deviance <- table(test$Class, predict_tree_deviance)
names(dimnames(conf_tree_deviance)) <- c("Actual Test", "Predicted Test")
caret::confusionMatrix(conf_tree_deviance)
```

```
## Confusion Matrix and Statistics
##
##            Predicted Test
## Actual Test  0  1
##           0 62 15
##           1  4 57
##
##                Accuracy : 0.8623
##                  95% CI : (0.7934, 0.915)
##     No Information Rate : 0.5217
##     P-Value [Acc > NIR] : < 2e-16
##
##                   Kappa : 0.726
##
##  Mcnemar's Test P-Value : 0.02178
##
##             Sensitivity : 0.9394
##             Specificity : 0.7917
##          Pos Pred Value : 0.8052
##          Neg Pred Value : 0.9344
##              Prevalence : 0.4783
##          Detection Rate : 0.4493
##    Detection Prevalence : 0.5580
##       Balanced Accuracy : 0.8655
##
```

```
##        'Positive' Class : 0
##
```

```
# plot of the tree
plot(tree_deviance)
text(tree_deviance)
```



Trees using rpart

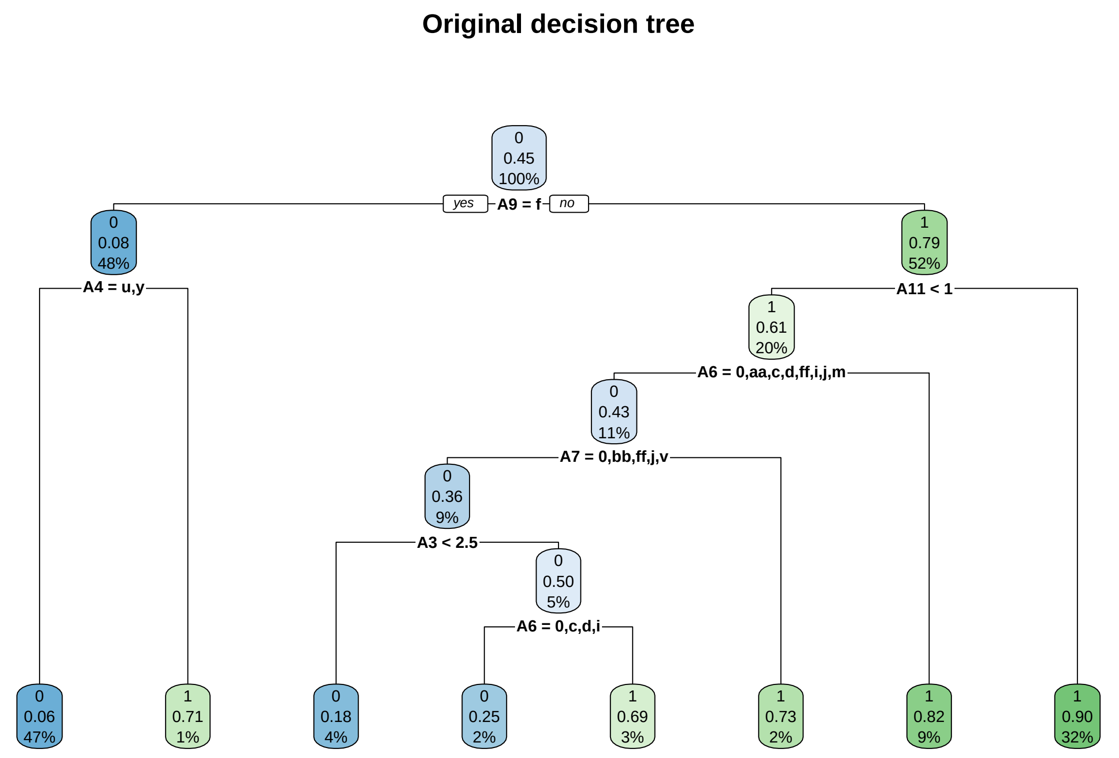
```
library(rpart.plot)
```

```
## Loading required package: rpart
```

```
##
## Attaching package: 'rpart'
```

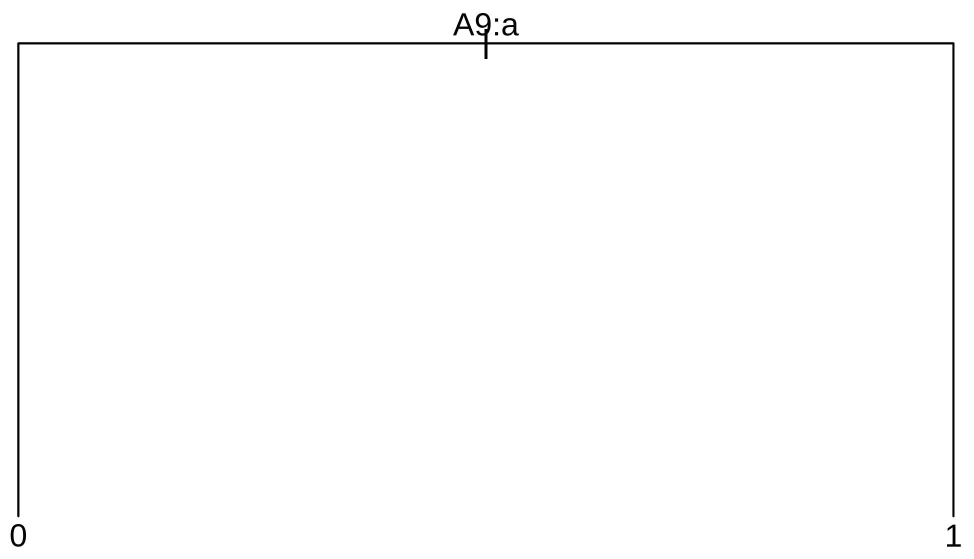
```
## The following object is masked from 'package:survival':
##
##     solder
```

```
library(rpart)

set.seed(12345)


decision_tree_rpart <- rpart::rpart(data = train, formula = Class~., method = "class")
rpart.plot::rpart.plot(decision_tree_rpart, main= "Original decision tree")
```

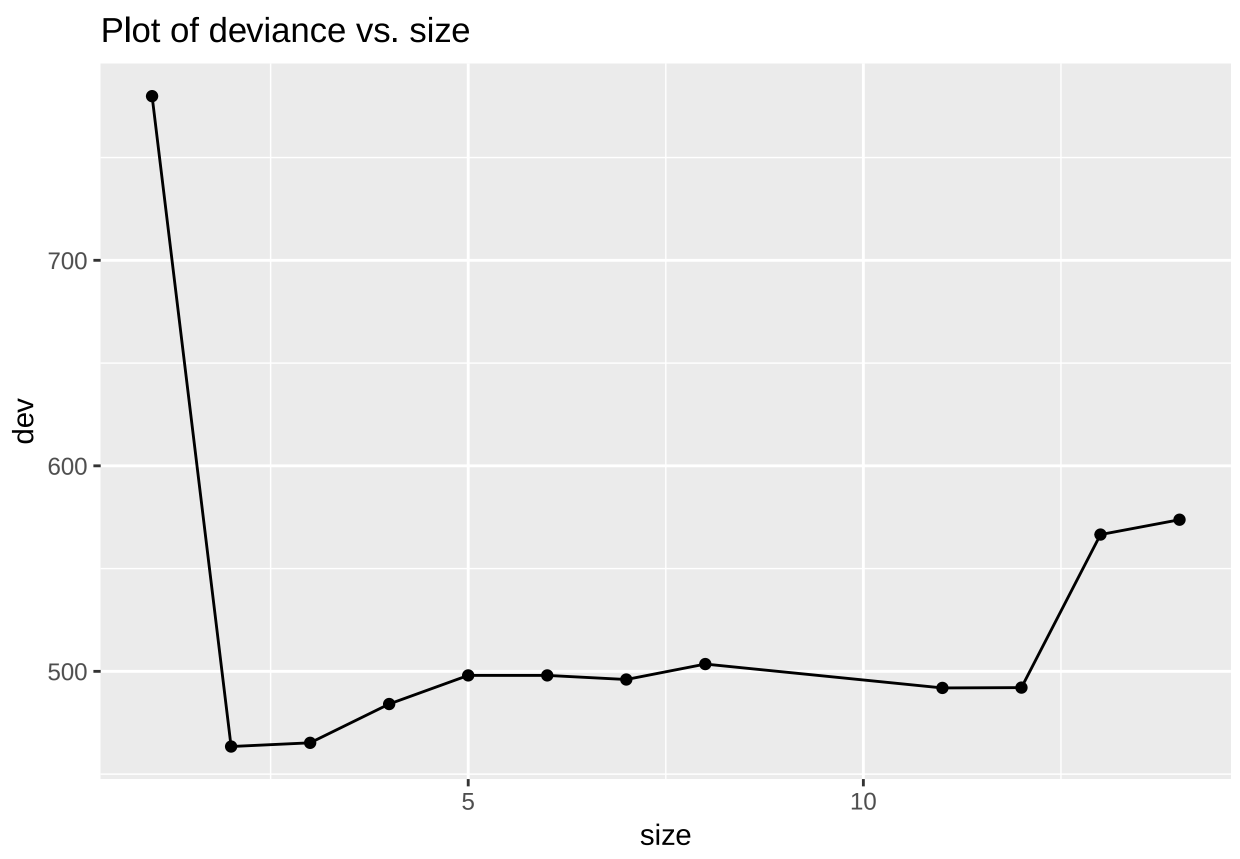


Pruning trees using cross validation

```
library(ggplot2)

set.seed(12345)
cv_tree <- cv.tree(tree_deviance, FUN = prune.tree, K = 10)
df_result <- as.data.frame(cbind(size = cv_tree$size, dev = cv_tree$dev))
# puring the tree for leaf size of 3
best_tree <- prune.tree(tree_deviance, best = 2)
plot(best_tree, main="Pruned Tree for the given dataset")
text(best_tree)
```

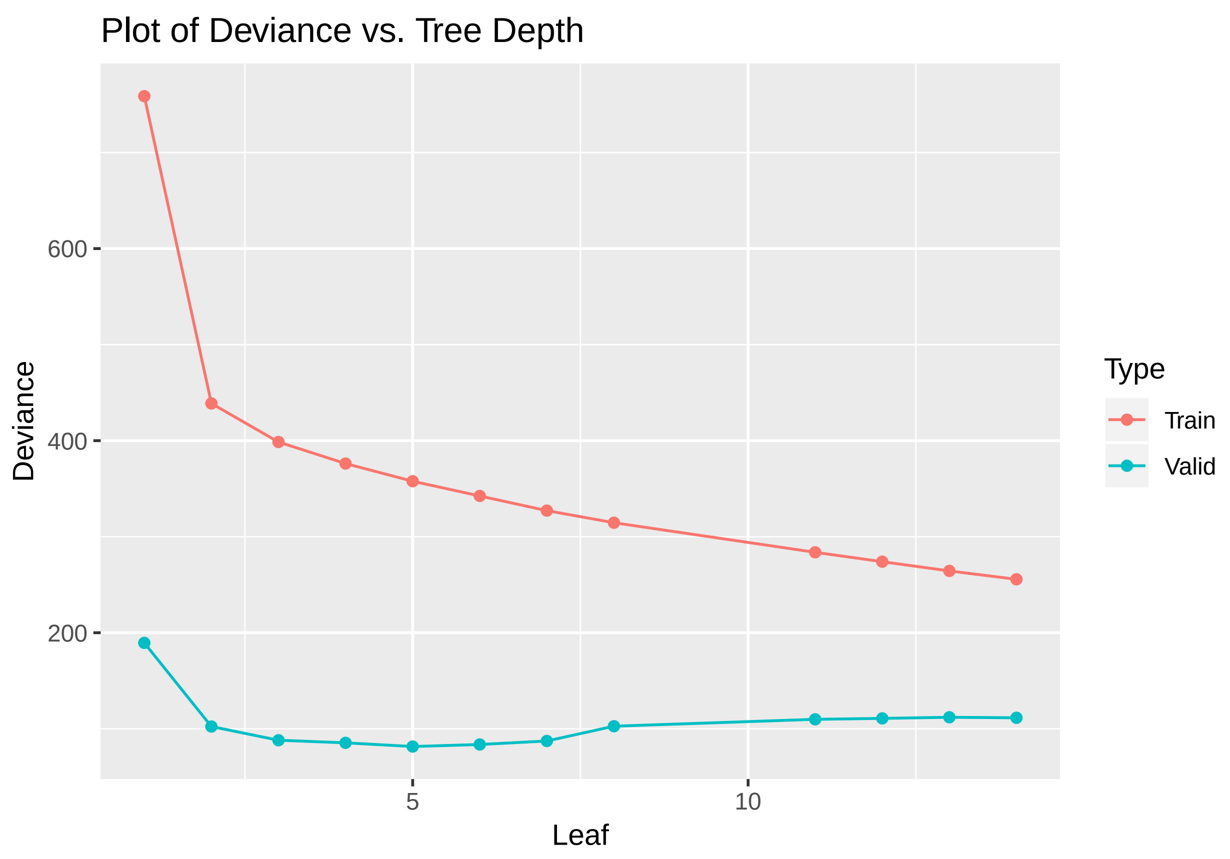


```
ggplot(df_result, aes(x = size, y = dev)) + geom_point() + geom_line() + ggtitle("Plot of deviance vs. s
```



Prune the tree using error

```
set.seed(12345)
tree_deviance <- tree::tree(Class~., data=train, split = c("deviance"))

tree_prune_train <- prune.tree(tree_deviance, method = c("deviance"))
tree_prune_valid <- prune.tree(tree_deviance, newdata = test ,method = c("deviance"))

result_train <- cbind(tree_prune_train$size,
tree_prune_train$dev, "Train")

result_valid <- cbind(tree_prune_valid$size,
tree_prune_valid$dev, "Valid")

result <- as.data.frame(rbind(result_valid, result_train))
colnames(result) <- c("Leaf", "Deviance", "Type")
result$Leaf <- as.numeric(as.character(result$Leaf))
result$Deviance <- as.numeric(as.character(result$Deviance))

# plot of deviance vs. number of leafs
ggplot(data = result, aes(x = Leaf, y = Deviance, colour = Type)) +
geom_point() + geom_line() +
ggtitle("Plot of Deviance vs. Tree Depth")
```

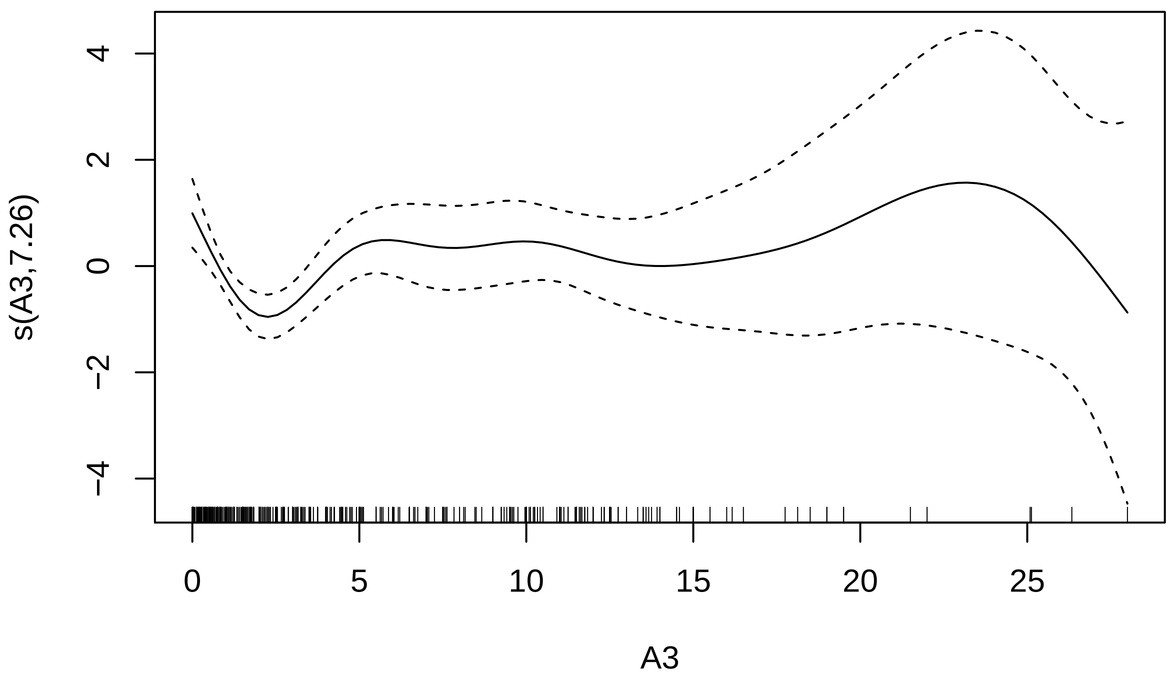


GAM Model or Spline

```r
set.seed(12345)

# using family = binomial for classfication
gam_model <- mgcv::gam(data=train, formula = Class~s(A3)+A9, family=binomial)
summary(gam_model)
```

```
##
## Family: binomial
## Link function: logit
##
## Formula:
## Class ~ s(A3) + A9
##
## Parametric coefficients:
##             Estimate Std. Error z value Pr(>|z|)
## (Intercept)  -2.6202     0.2479  -10.57   <2e-16 ***
## A9t           3.9741     0.3004   13.23   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Approximate significance of smooth terms:
##         edf Ref.df Chi.sq p-value
## s(A3) 7.264  8.259  22.28  0.0057 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## R-sq.(adj) =  0.525   Deviance explained = 45.7%
## UBRE = -0.22005  Scale est. = 1         n = 552
```

```
plot(gam_model)
```



```
# predicted the class, type="response" gives the probability, while if supported type="class" gives the
test$Predicted_Class_probability <- predict(object = gam_model, newdata=test, type = "response")
test$Predicted_Class <- ifelse(test$Predicted_Class_probability > 0.5, 1, 0)
```

Model Equation is given by Class = A9 + f(A3), where f is a smoothing function in our case determined by REML.

Use the following error function to compute the test error for the GAM and tree models, given by the below equation. Where Y is the actual class and Pi is the probability of predicted class being 1

$$E = \sum_i Y_i \cdot log(p_i) + (1 - Y_i) \cdot log(1 - P_i)$$

```
# Error-rate
error_rate = sum(as.numeric(test$Class) * log(test$Predicted_Class_probability) + (1 - as.numeric(test$

error_rate
```

```
## [1] -122.4911
```

Support Vector Machine (SVM)

```r
# width is the sigma here. kernel rbfdot is gaussian. vanilladot is linear
data(spam)
spam$type <- as.factor(spam$type)

## create test and training set
n=nrow(spam)
id=sample(1:n, floor(n*0.8))
spamtrain=spam[id,]
spamtest=spam[-id,]


model_0.05 <- kernlab::ksvm(type~., data=spamtrain, kernel="rbfdot", kpar=list(sigma=0.05), C=0.5)
#model_0.05

conf_model_0.05 <- table(spamtrain[,58], predict(model_0.05, spamtrain[,-58]))
names(dimnames(conf_model_0.05)) <- c("Actual Test", "Predicted Test")
caret::confusionMatrix(conf_model_0.05)
```

```
## Confusion Matrix and Statistics
##
##            Predicted Test
## Actual Test nonspam spam
##     nonspam    2174   52
##     spam        112 1342
##
##                Accuracy : 0.9554
##                  95% CI : (0.9483, 0.9619)
##     No Information Rate : 0.6212
##     P-Value [Acc > NIR] : < 2.2e-16
##
##                   Kappa : 0.9061
##
##  Mcnemar's Test P-Value : 4.083e-06
##
##             Sensitivity : 0.9510
##             Specificity : 0.9627
##          Pos Pred Value : 0.9766
##          Neg Pred Value : 0.9230
##              Prevalence : 0.6212
##          Detection Rate : 0.5908
##    Detection Prevalence : 0.6049
##       Balanced Accuracy : 0.9569
##
##        'Positive' Class : nonspam
##
```

ADA boost or Ensemble

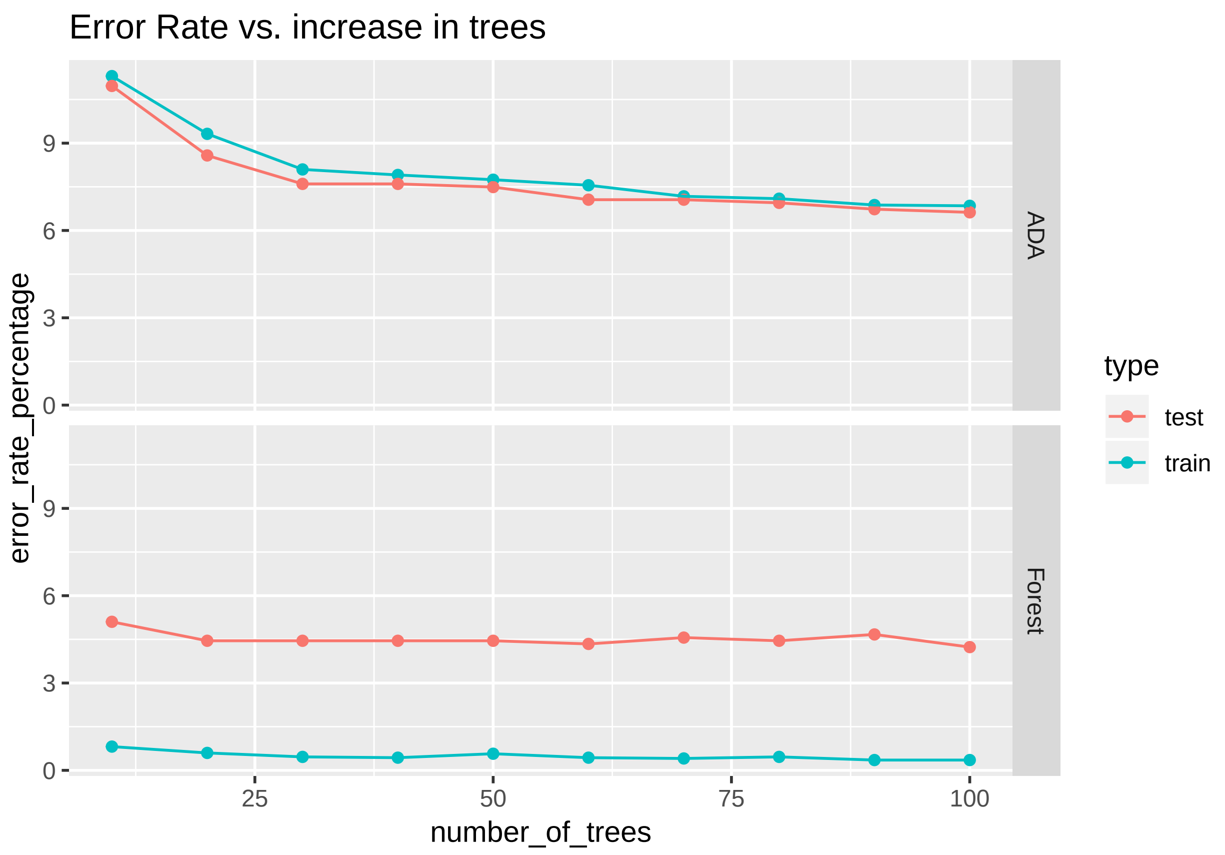
```r
data(spam)
## create test and training set
n=nrow(spam)
id=sample(1:n, floor(n*0.8))
spamtrain=spam[id,]
spamtest=spam[-id,]

ada_model <- mboost::blackboost(type~., data = spamtrain, family = AdaExp(),
                                control=boost_control(mstop=15))
test_ada_model_predict <- predict(ada_model, newdata = spamtest, type = c("class"))
```

Random Forest

```r
forest_model <- randomForest(type~., data = spamtrain, ntree = 15)
test_forest_model_predict <- predict(forest_model, newdata = spamtest, type = c("class"))
```

Comparing ADA boost and Randomforest

```r
# using warnings = FALSE

final_result <- NULL

for(i in seq(from = 10, to = 100, by = 10)){
ada_model <- mboost::blackboost(type~.,
data = spamtrain,
family = AdaExp(),
control=boost_control(mstop=i))

forest_model <- randomForest(type~., data = spamtrain, ntree = i)

prediction_function <- function(model, data){
predicted <- predict(model, newdata = data, type = c("class"))
predict_correct <- ifelse(data$type == predicted, 1, 0)
score <- sum(predict_correct)/NROW(data)
return(score)
}

train_ada_model_predict <- predict(ada_model, newdata = spamtrain, type = c("class"))
test_ada_model_predict <- predict(ada_model, newdata = spamtest, type = c("class"))
train_forest_model_predict <- predict(forest_model, newdata = spamtrain, type = c("class"))
test_forest_model_predict <- predict(forest_model, newdata = spamtest, type = c("class"))

test_predict_correct <- ifelse(spamtest$type == test_forest_model_predict, 1, 0)
train_predict_correct <- ifelse(spamtest$type == train_forest_model_predict, 1, 0)

train_ada_score <- prediction_function(ada_model, spamtrain)
test_ada_score <- prediction_function(ada_model, spamtest)
train_forest_score <- prediction_function(forest_model, spamtrain)
test_forest_score <- prediction_function(forest_model, spamtest)

iteration_result <- data.frame(number_of_trees = i,
accuracy = c(train_ada_score,
test_ada_score,
train_forest_score,
test_forest_score),
type = c("train", "test", "train", "test"),
model = c("ADA", "ADA", "Forest", "Forest"))
final_result <- rbind(iteration_result, final_result)
}

final_result$error_rate_percentage <- 100*(1 - final_result$accuracy)

ggplot(data = final_result, aes(x = number_of_trees,
y = error_rate_percentage,
group = type, color = type)) +
geom_point() +
geom_line() +
ggtitle("Error Rate vs. increase in trees") +
facet_grid(rows = vars(model))
```

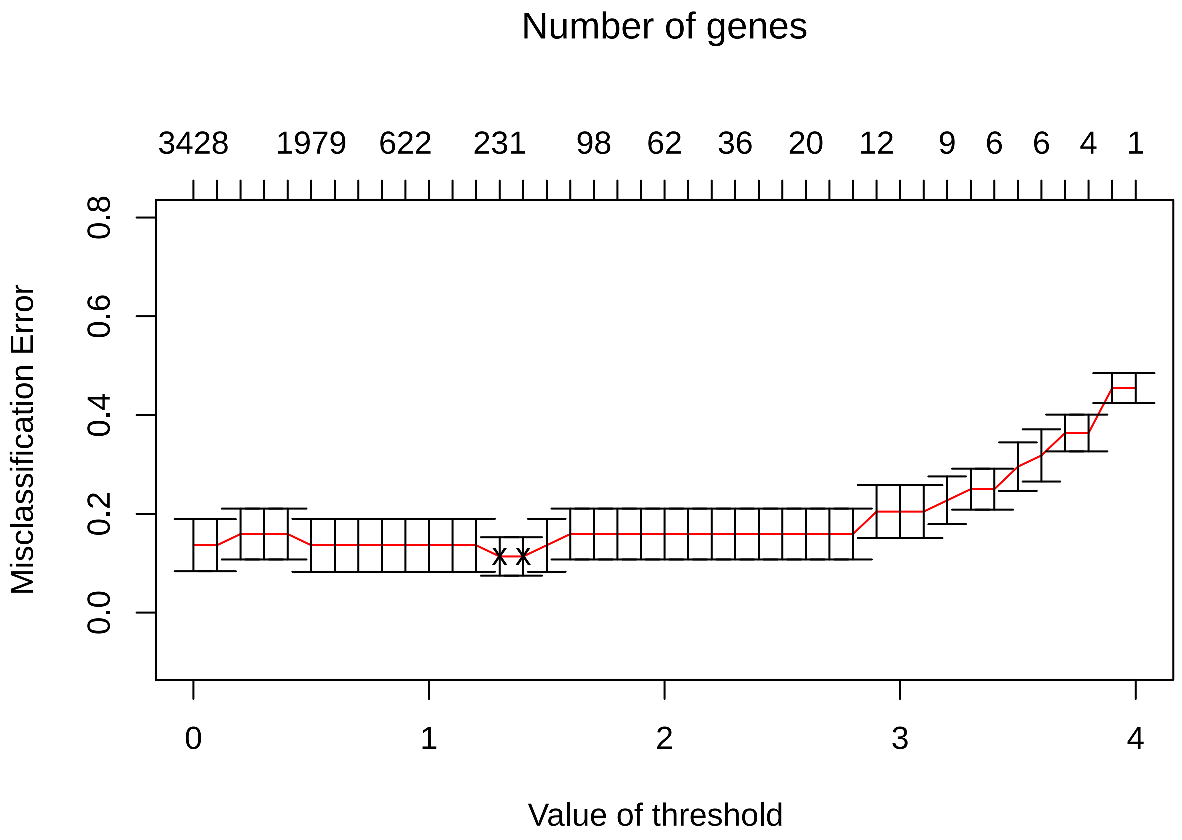


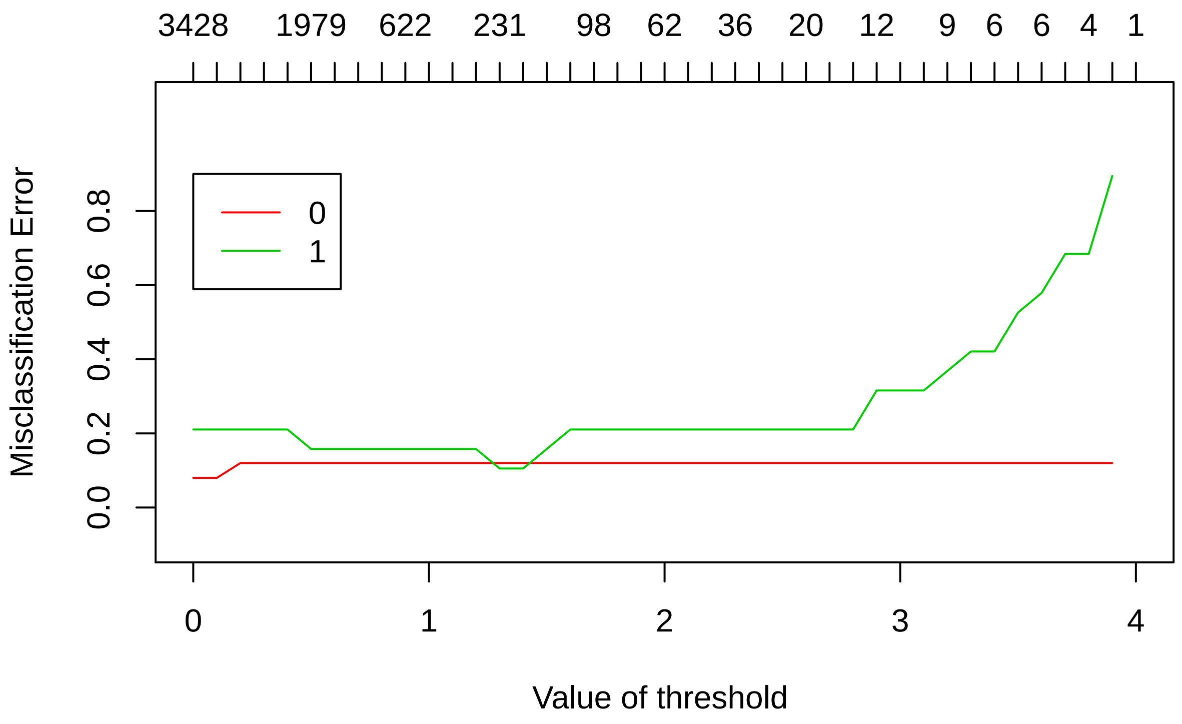
Nearest Shrunken Centroid (NSC)

```r
data <- read.csv(file = "data.csv", sep = ";", header = TRUE)
n=NROW(data)
data$Conference <- as.factor(data$Conference)


# Remember to scale the data, its cruical for this algorithm, like so scale_data = scale(data)

set.seed(12345)
id=sample(1:n, floor(n*0.7))
train=data[id,]
test = data[-id,]

rownames(train)=1:nrow(train)
x=t(train[,-4703])
y=train[[4703]]

rownames(test)=1:nrow(test)
x_test=t(test[,-4703])
y_test=test[[4703]]

mydata = list(x=x,y=as.factor(y),geneid=as.character(1:nrow(x)), genenames=rownames(x))
mydata_test = list(x=x_test,y=as.factor(y_test),geneid=as.character(1:nrow(x)), genenames=rownames(x))
model=pamr.train(mydata,threshold=seq(0, 4, 0.1))

cvmodel=pamr.cv(model, mydata)

# The value at which loglikehood is max, we can use this or use the threshold for which error is least
cvmodel$threshold[which.max(cvmodel$loglik)]


important_gen <- as.data.frame(pamr.listgenes(model, mydata, threshold = 1.3))
predicted_scc_test <- pamr.predict(model, newx = x_test, threshold = 1.3)
```

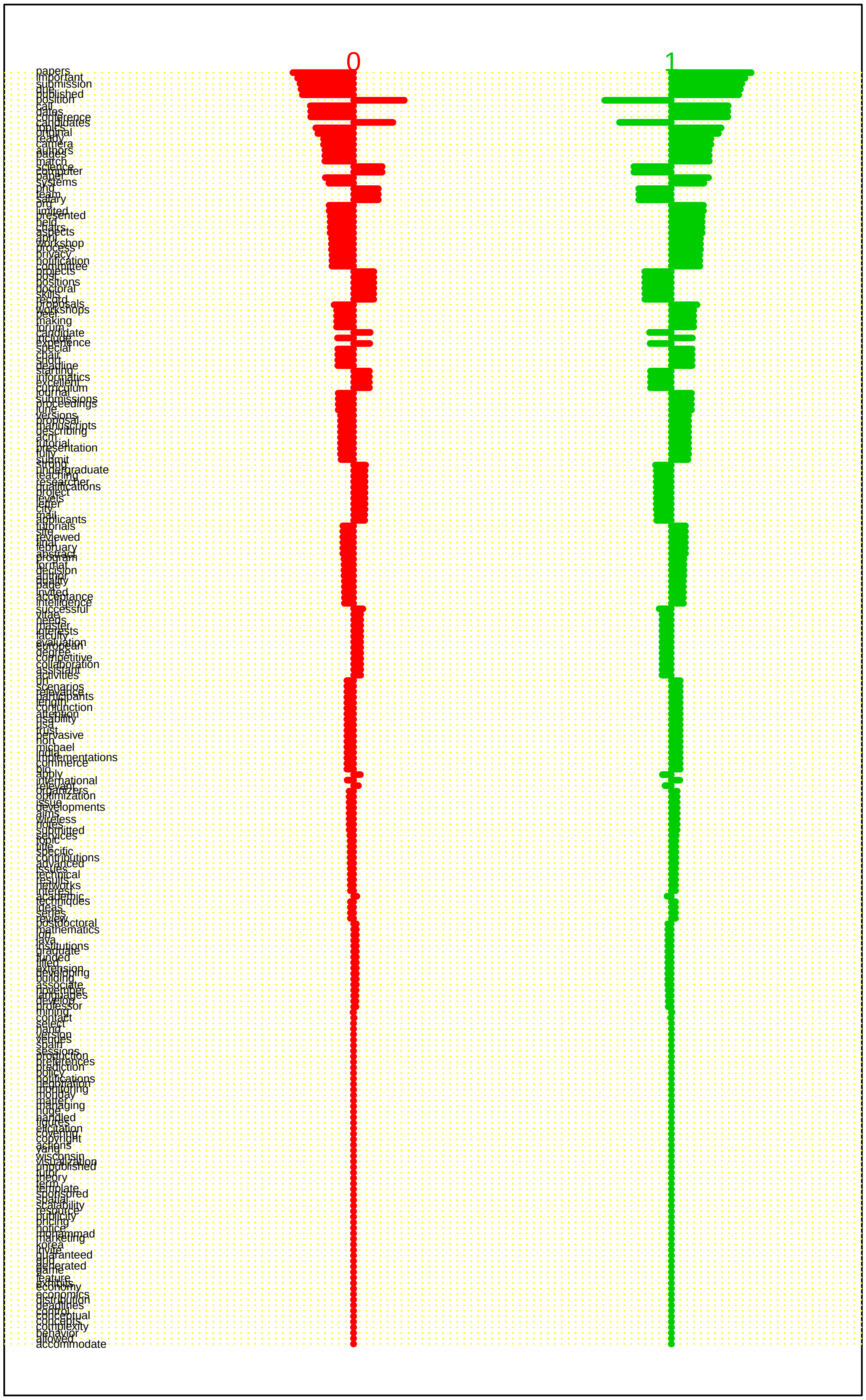
Plots

```r
# use {r, fig.height=9} for better plots
pamr.plotcv(cvmodel)
```


Number of genes
3428 1979 622 231 98 62 36 20 12 9 6 6 4 1
Misclassification Error
0.0 0.2 0.4 0.6 0.8
0 1 2 3 4
Value of threshold


3428 1979 622 231 98 62 36 20 12 9 6 6 4 1
Misclassification Error
0.0 0.2 0.4 0.6 0.8
0
1
0 1 2 3 4
Value of threshold

```r
pamr.plotcen(model, mydata, threshold = 1.3)
```



0
1
papers
important
submission
published
position
dates
conference
candidates
original
camera
authors
pages
match
science
computer
systems
phd
team
salary
limited
presented
aspects
workshop
privacy
notification
committee
projects
positions
doctoral
proposals
workshops
making
forum
candidate
experience
special
chair
deadline
informatics
excellent
curriculum
journal
submissions
proceedings
versions
proposal
participants
describing
tutorial
presentation
fully
submit
undergraduate
teaching
researcher
qualifications
project
levels
letter
city
applicants
tutorials
reviewed
february
abstracts
program
format
decision
invited
acceptance
intelligence
successful
interests
faculty
evaluation
european
degree
competitive
collaboration
assistant
activities
scenarios
relevance
participants
conjunction
attention
usability
usa
pervasive
michael
implementations
commerce
apply
international
optimization
developments
wireless
submitted
services
topic
specific
contributions
advanced
issues
technical
results
networks
interest
academic
techniques
ideas
series
review
postdoctoral
mathematics
institutions
graduate
funded
extension
building
associate
languages
professor
mining
contact
select
version
venues
sessions
production
preferences
prediction
policy
notifications
monitoring
managing
handled
excitation
copyright
actions
wisconsin
visualization
unpublished
theory
term
template
sponsored
scalability
publicity
pricing
notice
mohammad
marketing
korea
guaranteed
generated
game
feature
economy
economics
distribution
deadlines
conceptual
complexity
behavior
allowed
accommodate

Important features

```
## List the significant genes
NROW(important_gen)
```

```
## [1] 231
```

```
temp <- colnames(data) %>% as.data.frame()
colnames(temp) <- "col_name"
temp$index <- row.names(temp)

df <- merge(x = important_gen, y = temp, by.x = "id", by.y = "index", all.x = TRUE)
df <- df[order(df[,3], decreasing = TRUE ),]

knitr::kable(head(df[,4],10), caption = "Important feaures selected by Nearest Shrunken Centroids ")
```

Table 1: Important feaures selected by Nearest Shrunken Centroids

x
papers
important
submission
due
published
call
dates
conference
topics
original

Confusion table

```
conf_scc <- table(y_test, predicted_scc_test)
names(dimnames(conf_scc)) <- c("Actual Test", "Predicted Srunken Centroid Test")
result_scc <- caret::confusionMatrix(conf_scc)
caret::confusionMatrix(conf_scc)
```

```
## Confusion Matrix and Statistics
##
##            Predicted Srunken Centroid Test
## Actual Test  0  1
##           0 10  0
##           1  2  8
##
##                Accuracy : 0.9
##                  95% CI : (0.683, 0.9877)
##     No Information Rate : 0.6
##     P-Value [Acc > NIR] : 0.003611
##
##                   Kappa : 0.8
##
##  Mcnemar's Test P-Value : 0.479500
```

```
##
##             Sensitivity : 0.8333
##             Specificity : 1.0000
##          Pos Pred Value : 1.0000
##          Neg Pred Value : 0.8000
##              Prevalence : 0.6000
##          Detection Rate : 0.5000
##    Detection Prevalence : 0.5000
##       Balanced Accuracy : 0.9167
##
##        'Positive' Class : 0
##
```

Elastic Net

```
x = train[,-4703] %>% as.matrix()
y = train[,4703]

x_test = test[,-4703] %>% as.matrix()
y_test = test[,4703]

cvfit = cv.glmnet(x=x, y=y, alpha = 0.5, family =   "binomial")
predicted_elastic_test <- predict.cv.glmnet(cvfit, newx = x_test, s = "lambda.min", type = "class")
tmp_coeffs <- coef(cvfit, s = "lambda.min")
elastic_variable <- data.frame(name = tmp_coeffs@Dimnames[[1]][tmp_coeffs@i + 1], coefficient = tmp_coe
knitr::kable(elastic_variable, caption = "Contributing features in the elastic model")
```

Table 2: Contributing features in the elastic model

name	coefficient
(Intercept)	-1.0189313
abstracts	-0.3011264
aspects	0.0736776
bio	0.0228765
call	0.3319900
candidates	-0.1878311
computer	-0.2832065
conceptual	0.0380844
conference	0.1965330
dates	0.2416630
due	0.5211725
evaluation	-0.1796401
exhibits	0.3782700
important	0.3924275
languages	-0.0258470
making	0.1892394
manuscripts	0.0325584
original	0.0558205
papers	0.3853810
peer	0.0967211
position	-0.3750830
process	0.0016238

name	coefficient
projects	-0.1904080
proposals	0.0553554
published	0.2818206
queries	-0.3002459
record	-0.1162514
relevant	-0.1135564
scenarios	0.0053470
spatial	0.1925007
submission	0.2803519
team	-0.1291278
versions	0.1545749

```
conf_elastic_net <- table(y_test, predicted_elastic_test)
names(dimnames(conf_elastic_net)) <- c("Actual Test", "Predicted ElasticNet Test")
result_elastic_net <- caret::confusionMatrix(conf_elastic_net)
caret::confusionMatrix(conf_elastic_net)
```

```
## Confusion Matrix and Statistics
##
##            Predicted ElasticNet Test
## Actual Test  0  1
##           0 10  0
##           1  2  8
##
##                Accuracy : 0.9
##                  95% CI : (0.683, 0.9877)
##     No Information Rate : 0.6
##     P-Value [Acc > NIR] : 0.003611
##
##                   Kappa : 0.8
##
##  Mcnemar's Test P-Value : 0.479500
##
##             Sensitivity : 0.8333
##             Specificity : 1.0000
##          Pos Pred Value : 1.0000
##          Neg Pred Value : 0.8000
##              Prevalence : 0.6000
##          Detection Rate : 0.5000
##    Detection Prevalence : 0.5000
##       Balanced Accuracy : 0.9167
##
##        'Positive' Class : 0
##
```

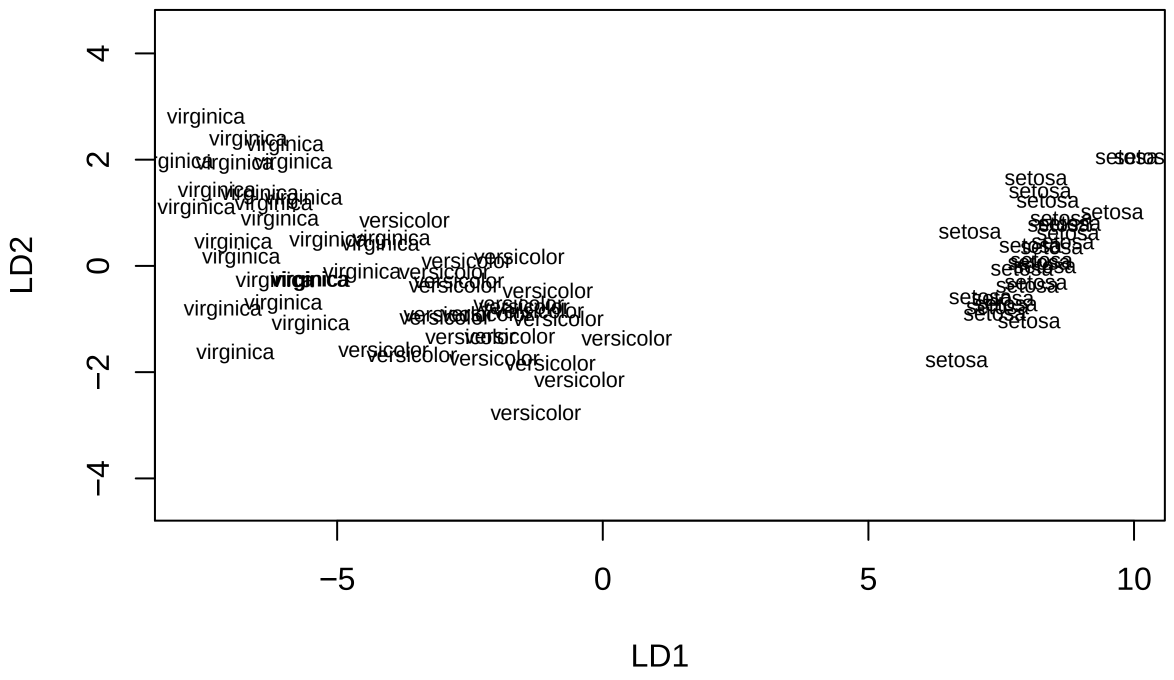
Linear discriminant analysis (LDA)

```
# Load the data
data <- iris
# Split the data into training (80%) and test set (20%)
```

```
n=NROW(data)
set.seed(12345)
id=sample(1:n, floor(n*0.5))
train=data[id,]
test=data[-id,]

model <- MASS::lda(Species~., data = train)
model
```

```
## Call:
## lda(Species ~ ., data = train)
##
## Prior probabilities of groups:
##     setosa versicolor  virginica
##  0.3600000  0.3066667  0.3333333
##
## Group means:
##            Sepal.Length Sepal.Width Petal.Length Petal.Width
## setosa         5.007407    3.425926     1.481481    0.237037
## versicolor     5.986957    2.752174     4.317391    1.330435
## virginica      6.672000    3.064000     5.592000    2.060000
##
## Coefficients of linear discriminants:
##                     LD1        LD2
## Sepal.Length  0.4600007  0.4122668
## Sepal.Width   1.4530509  2.0465774
## Petal.Length -2.5357940 -1.4106421
## Petal.Width  -2.3130581  3.4312099
##
## Proportion of trace:
##    LD1    LD2
## 0.9882 0.0118
```

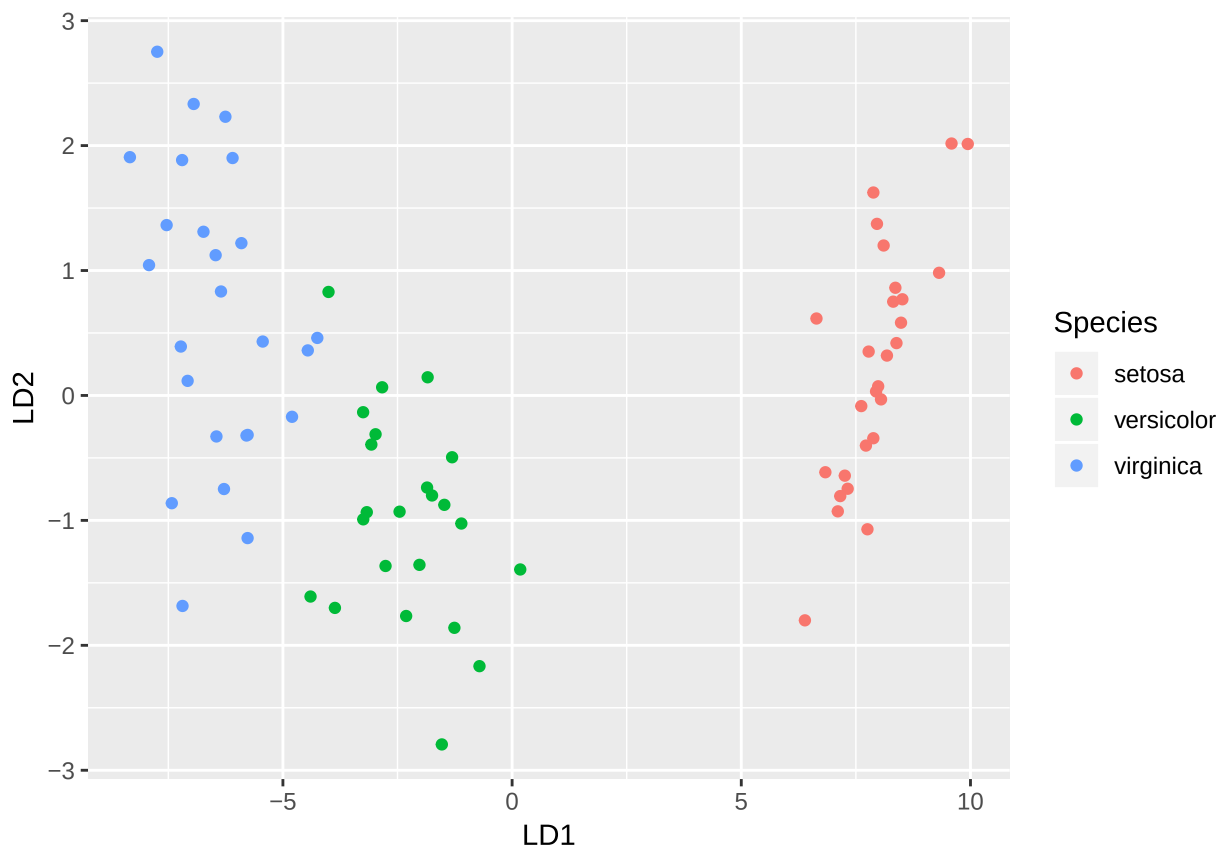
```
plot(model)
```



```
predictions <- model %>% predict(test)
names(predictions)
```

```
## [1] "class"     "posterior" "x"
```

```
lda.data <- cbind(train, predict(model)$x)
#plot(data2$frames,data2$duration, col=predict(m3)$class)

ggplot(lda.data, aes(LD1, LD2)) + geom_point(aes(color = Species))
```



Bootstrap and Big data

Principle Component Analysis

Components

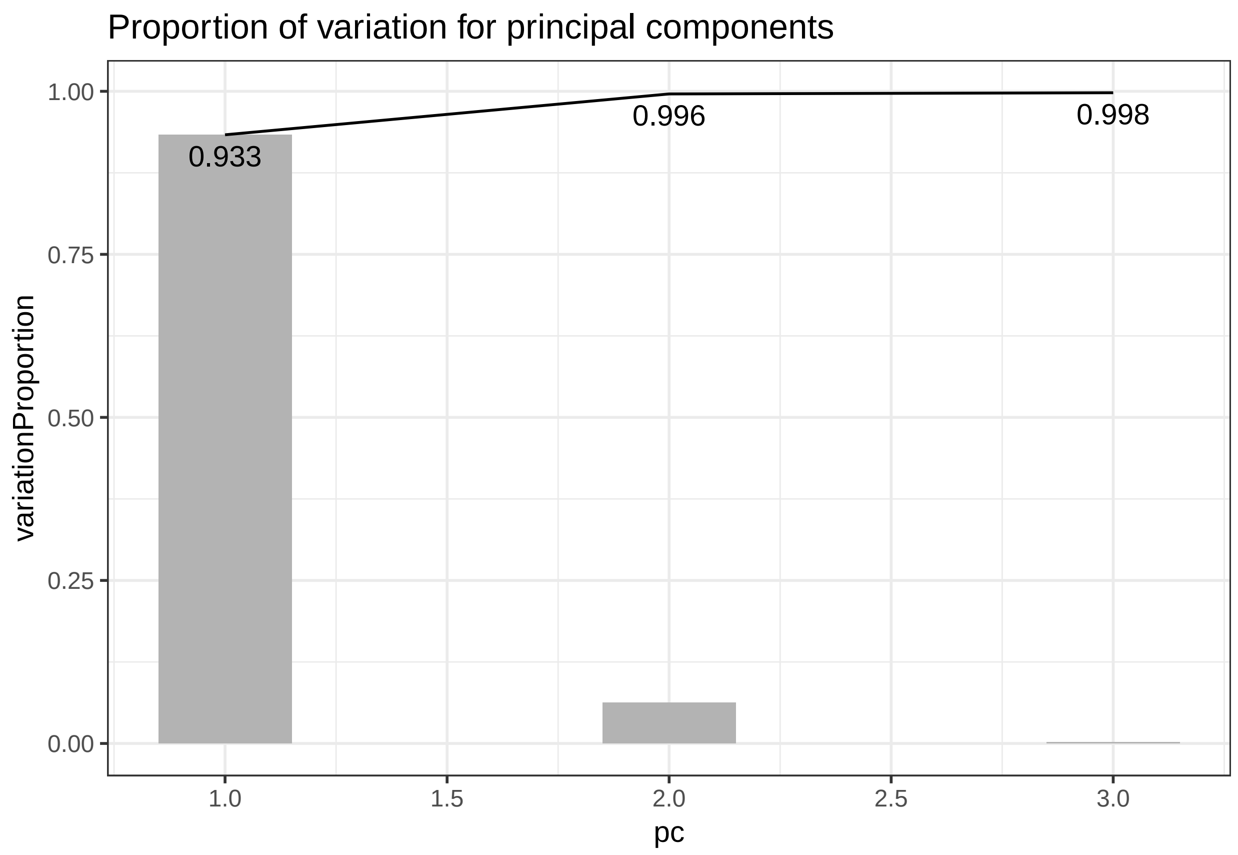
```
rm(list=ls())

set.seed(12345)
NIR_data <- read.csv2("NIRSpectra.csv")

## scaling is necessary else the column with high range will dominate, using prcomp(scale=TRUE)
pca_data =  select(NIR_data,-c(Viscosity))
pca_result = prcomp(pca_data)

contribution <- summary(pca_result)$importance
knitr::kable(contribution[,1:5],
             caption = "Contribution of PCA axis towards varience explaination")
```

Table 3: Contribution of PCA axis towards varience explaination

	PC1	PC2	PC3	PC4	PC5
Standard deviation	0.122062	0.0316205	0.0054353	0.0040107	0.0033031

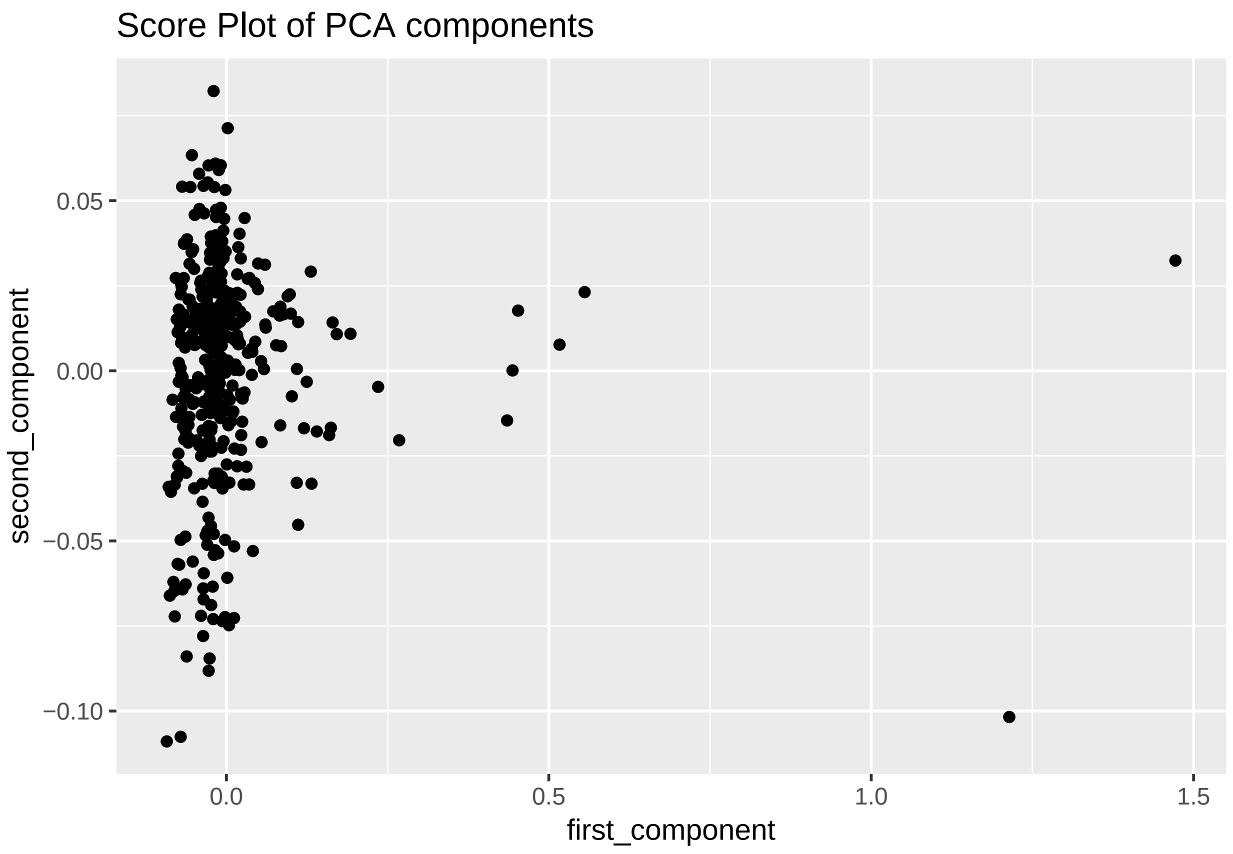
	PC1	PC2	PC3	PC4	PC5
Proportion of Variance	0.933320	0.0626300	0.0018500	0.0010100	0.0006800
Cumulative Proportion	0.933320	0.9959600	0.9978100	0.9988200	0.9995000

```r
eigenvalues = pca_result$sdev^2

# plotting proportion of variation for principal components
plotData = as.data.frame(cbind(pc = 1:3,
variationProportion = eigenvalues[1:3]/sum(eigenvalues),
cummulative = cumsum(eigenvalues[1:3]/sum(eigenvalues))))

ggplot(data = plotData) +
geom_col(aes(x = pc, y = variationProportion), width = 0.3, fill = "grey70") +
geom_line(data = plotData,
aes(x = pc, y = cummulative)) +
geom_text(aes(x = pc, y = cummulative, label = round(cummulative, 3)), size = 4,
position = "identity", vjust = 1.5) +
theme_bw() +
ggtitle("Proportion of variation for principal components")
```

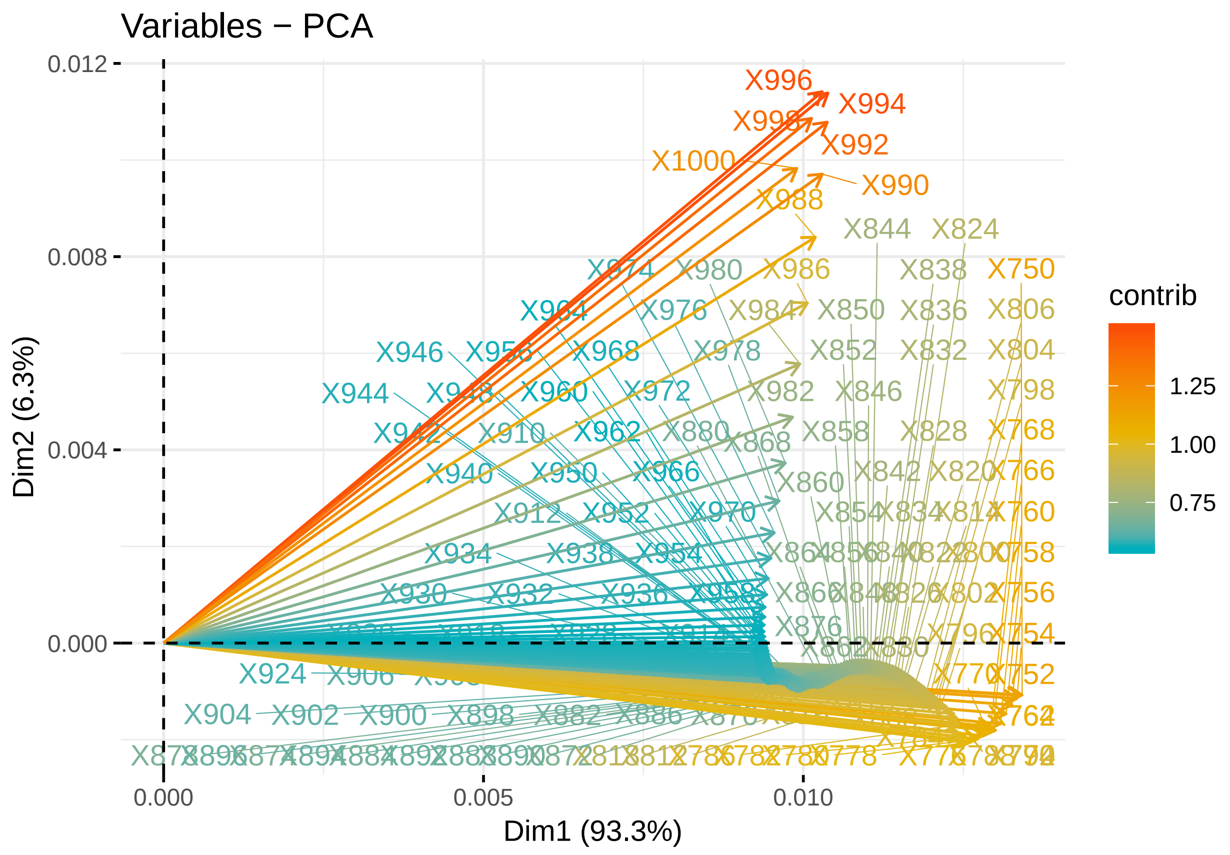


```r
# pca components and the viscocity
pca_result_data = cbind(first_component = pca_result$x[,1],
                                       second_component = pca_result$x[,2]) %>% as.data.frame()

# plotting the data variation and the viscocity
```

```
ggplot(data = pca_result_data, aes(x = first_component, y = second_component)) +
  geom_point() + ggtitle("Score Plot of PCA components")
```

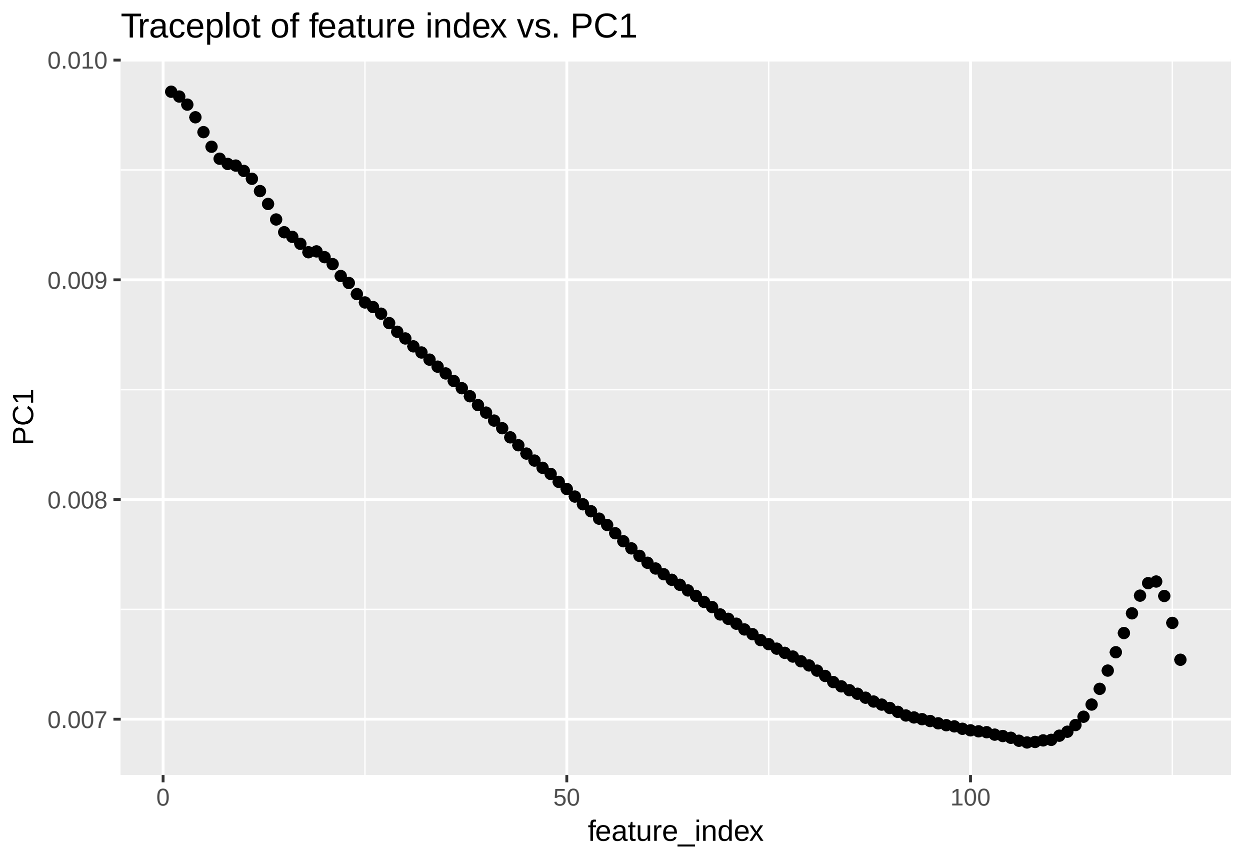


```
# showing the score of PCA component
factoextra::fviz_pca_var(pca_result,
             col.var = "contrib", # Color by contributions to the PC
             gradient.cols = c("#00AFBB", "#E7B800", "#FC4E07"),
             repel = TRUE     # Avoid text overlapping
             )
```

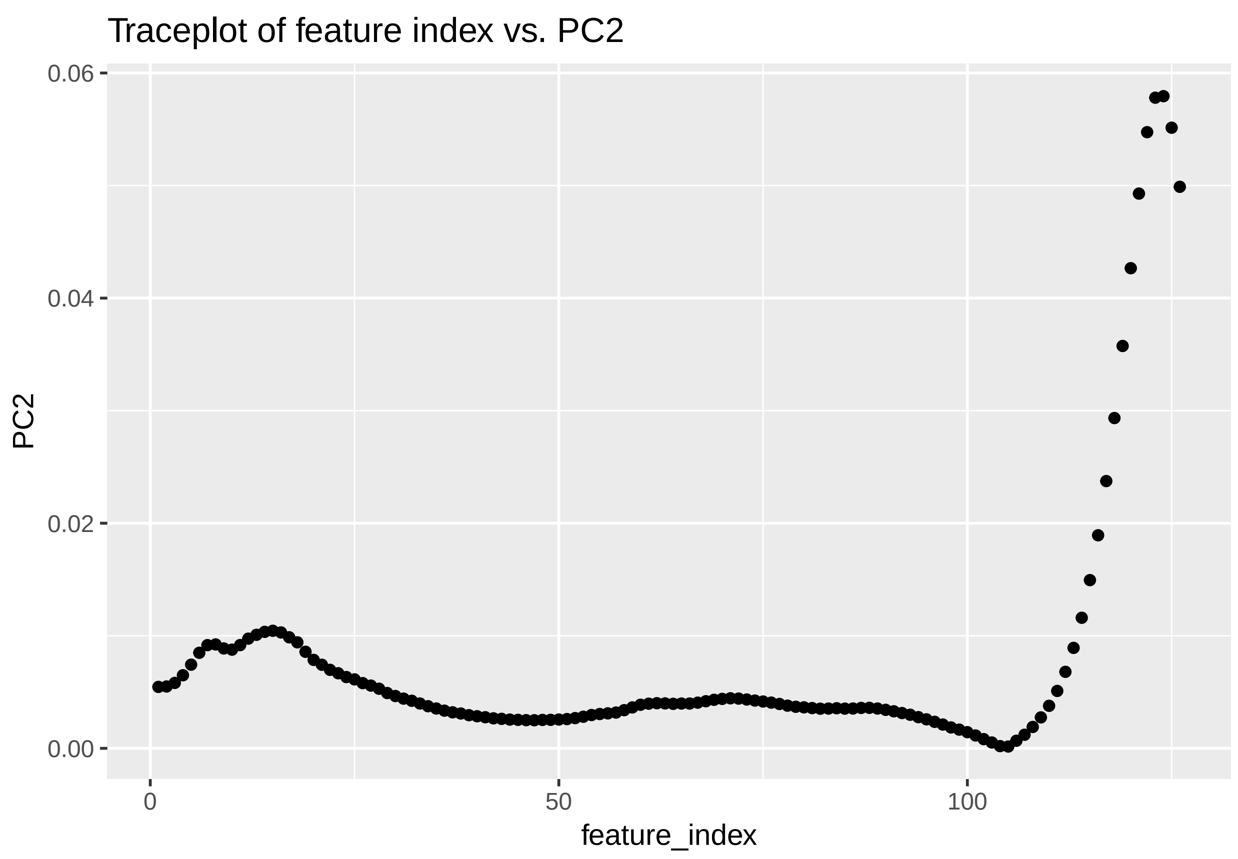


Trace plots of PCA

```
set.seed(12345)

# creating extra columns
aload <- abs(pca_result$rotation[,1:2])
components <- sweep(aload, 2, colSums(aload), "/")
components <- as.data.frame(components)
components$feature_name <- rownames(components)
components$feature_index <- 1:nrow(components)

ggplot(data = components, aes(x = feature_index, y = PC1)) +
  geom_point() +
  ggtitle("Traceplot of feature index vs. PC1")
```



```r
ggplot(data = components, aes(x = feature_index, y = PC2)) +
  geom_point() +
  ggtitle("Traceplot of feature index vs. PC2")
```



```r
knitr::kable(components[1:10,],
             caption = "Contribution of Features towards the Principle Components")
```

Table 4: Contribution of Features towards the Principle Components

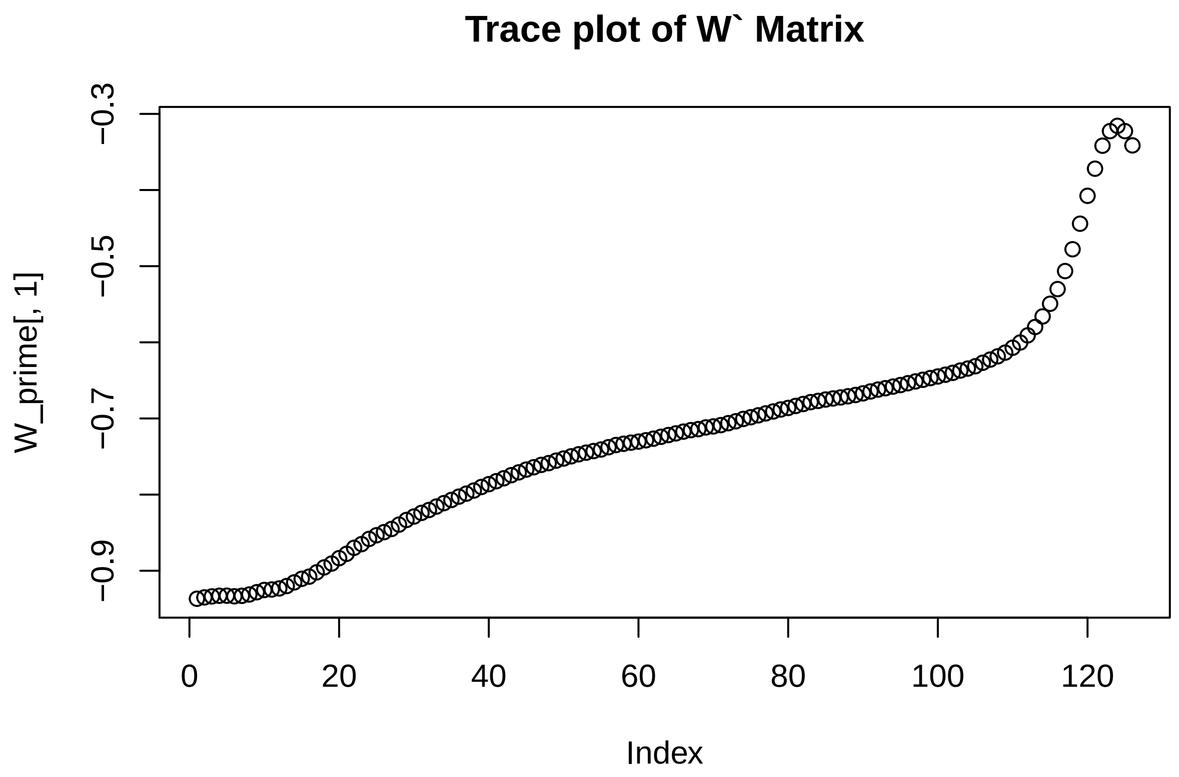
	PC1	PC2	feature_name	feature_index
X750	0.0098560	0.0054568	X750	1
X752	0.0098341	0.0054945	X752	2
X754	0.0097973	0.0058118	X754	3
X756	0.0097397	0.0064942	X756	4
X758	0.0096720	0.0074338	X758	5
X760	0.0096057	0.0084896	X760	6
X762	0.0095511	0.0091662	X762	7
X764	0.0095275	0.0092284	X764	8
X766	0.0095199	0.0088733	X766	9
X768	0.0094956	0.0087674	X768	10

FastICA

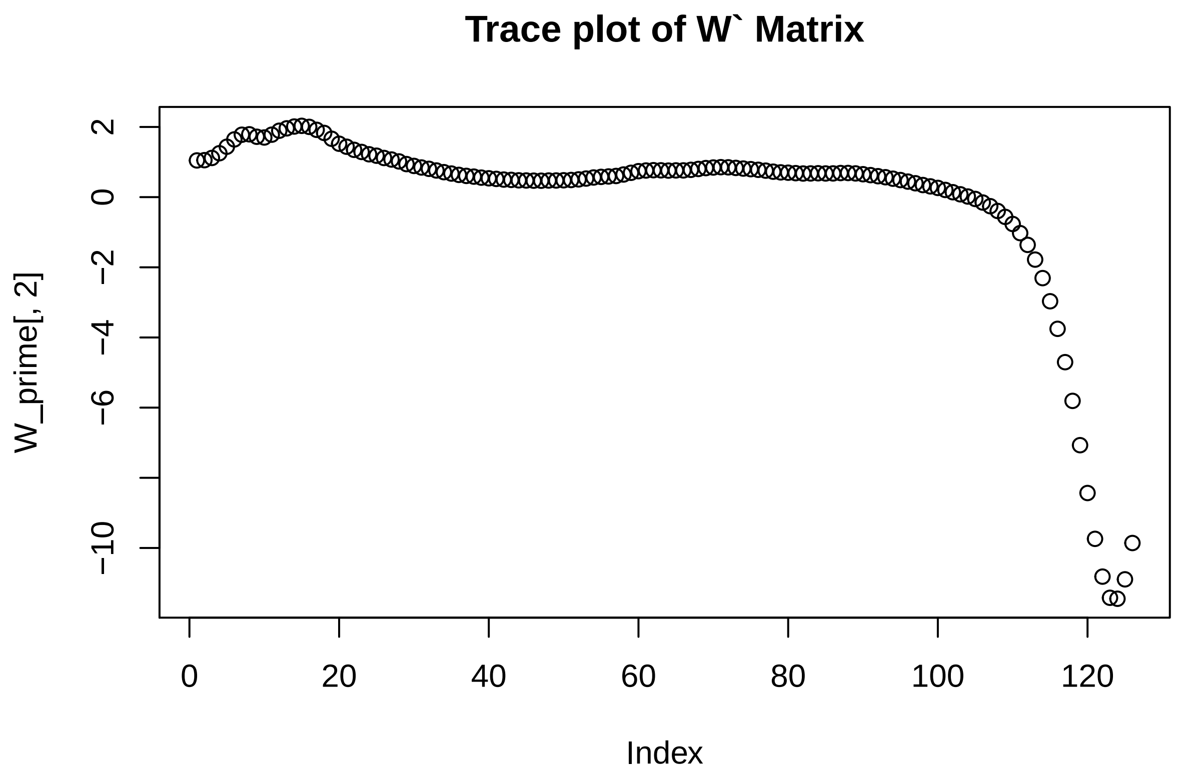
```r
library(fastICA)

set.seed(12345)

# X -> pre-processed data matrix
# K -> pre-whitening matrix that projects data onto the first n.compprincipal components.
# W -> estimated un-mixing matrix (see definition in details)
# A -> estimated mixing matrix
# S -> estimated source matrix

X <- as.matrix(pca_data)

ICA_extraction <- fastICA(X, 2, alg.typ = "parallel", fun = "logcosh", alpha = 1,
method = "R", row.norm = FALSE, maxit = 200,
tol = 0.0001, verbose = TRUE)
```

```
## Centering

## Whitening

## Symmetric FastICA using logcosh approx. to neg-entropy function

## Iteration 1 tol = 0.01930239

## Iteration 2 tol = 0.01303959

## Iteration 3 tol = 0.002393582

## Iteration 4 tol = 0.0006708454

## Iteration 5 tol = 0.0001661602

## Iteration 6 tol = 3.521604e-05
```

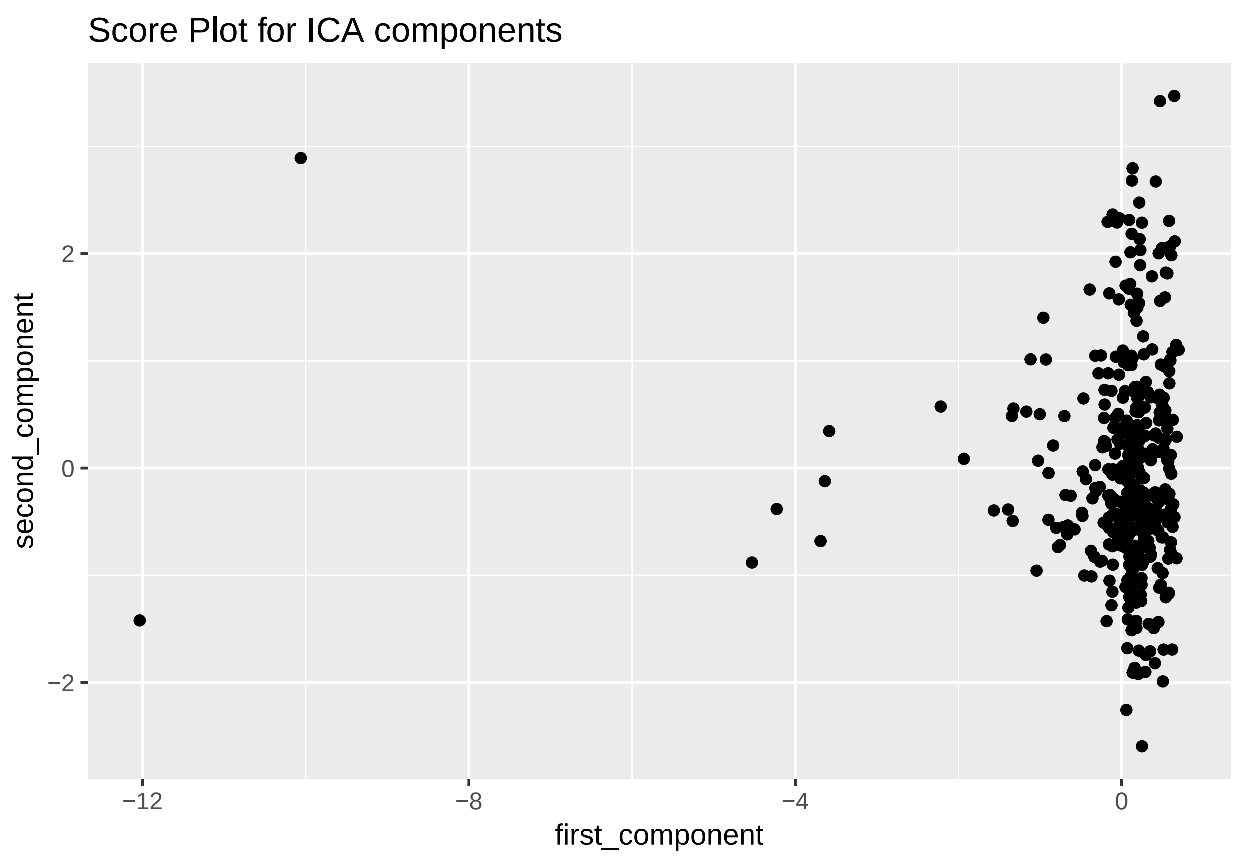
```r
W_prime <- ICA_extraction$K %*% ICA_extraction$W

#trace plots
plot(W_prime[,1], main = "Trace plot of W` Matrix")
```



```
#trace plots
plot(W_prime[,2], main = "Trace plot of W` Matrix")
```



```
# pca components and the viscocity
ICA_result_data = cbind(first_component = ICA_extraction$S[,1],
                        second_component = ICA_extraction$S[,2],
                        Viscosity = NIR_data$Viscosity) %>% as.data.frame()

# plotting the data variation
ggplot(data = ICA_result_data, aes(x = first_component, y = second_component)) +
  geom_point() + ggtitle("Score Plot for ICA components")
```



Implement Benjamini-Hochberg method

```
# function to compute the BH method on a dataframe
data <- read.csv("Influenza.csv")
new_data <- data %>% filter(Year > 1994 & Year < 1997)

x <- new_data %>% select(-c("Year"))
y <- new_data %>% select(c("Year"))
y <- factor(y$Year)

#initialzing the dataframe
p_values <- data.frame(feature = '',P_value = 0,stringsAsFactors = FALSE)

for(i in 1:ncol(x)){
  res = t.test(x[,i]~y, data = new_data, alternative="two.sided", conf.level = 0.95)
  p_values[i,] <- c(colnames(x)[i],res$p.value)
}

manual_BH_df = function(data, fpr) {
  data2 <- data %>%
    mutate(BH=p.adjust(P_value, "BH")) %>%
    arrange(P_value) %>%
    mutate(j = rank(P_value), m = n()) %>%
    mutate(BHmanual_base = j/m) %>%
    mutate(BHmanual_alpha = 0.15 * j / m,
           BHsignif_alpha = BHmanual_alpha <= fpr)

  return(data2)
}

manual_BH_df(data=p_values, fpr=0.05)
```

```
##                 feature            P_value         BH j m BHmanual_base BHmanual_alpha BHsignif_alpha
## 1             Temp_lag2 0.0115236887215172 0.09218951 1 8         0.125        0.01875           TRUE
## 2             Temp_lag1 0.0420408154818533 0.16816326 2 8         0.250        0.03750           TRUE
## 3             Influenza  0.200156779620115 0.47397535 3 8         0.375        0.05625          FALSE
## 4 Temperature.deficit  0.236987673201419 0.47397535 4 8         0.500        0.07500          FALSE
## 5        Influenza_lag2   0.50765830191299 0.79266727 5 8         0.625        0.09375          FALSE
## 6        Influenza_lag1  0.594500451143646 0.79266727 6 8         0.750        0.11250          FALSE
## 7             Mortality  0.977326166688916 1.00000000 7 8         0.875        0.13125          FALSE
## 8                  Week                  1 1.00000000 8 8         1.000        0.15000          FALSE
```

```
# alternative
data <- read.csv(file = "data.csv", sep = ";", header = TRUE)
data$Conference <- as.factor(data$Conference)
set.seed(12345)
y <- as.factor(data[,4703])
x <- as.matrix(data[,-4703])
p_values <- data.frame(feature = '',P_value = 0,stringsAsFactors = FALSE)
for(i in 1:ncol(x)){
res = t.test(x[,i]~y, data = data,
alternative="two.sided"
,conf.level = 0.95)
p_values[i,] <- c(colnames(x)[i],res$p.value)
}
p_values$P_value <- as.numeric(p_values$P_value)
p <- p.adjust(p_values$P_value, method = 'BH')
length(p[which(p > 0.05)])
```

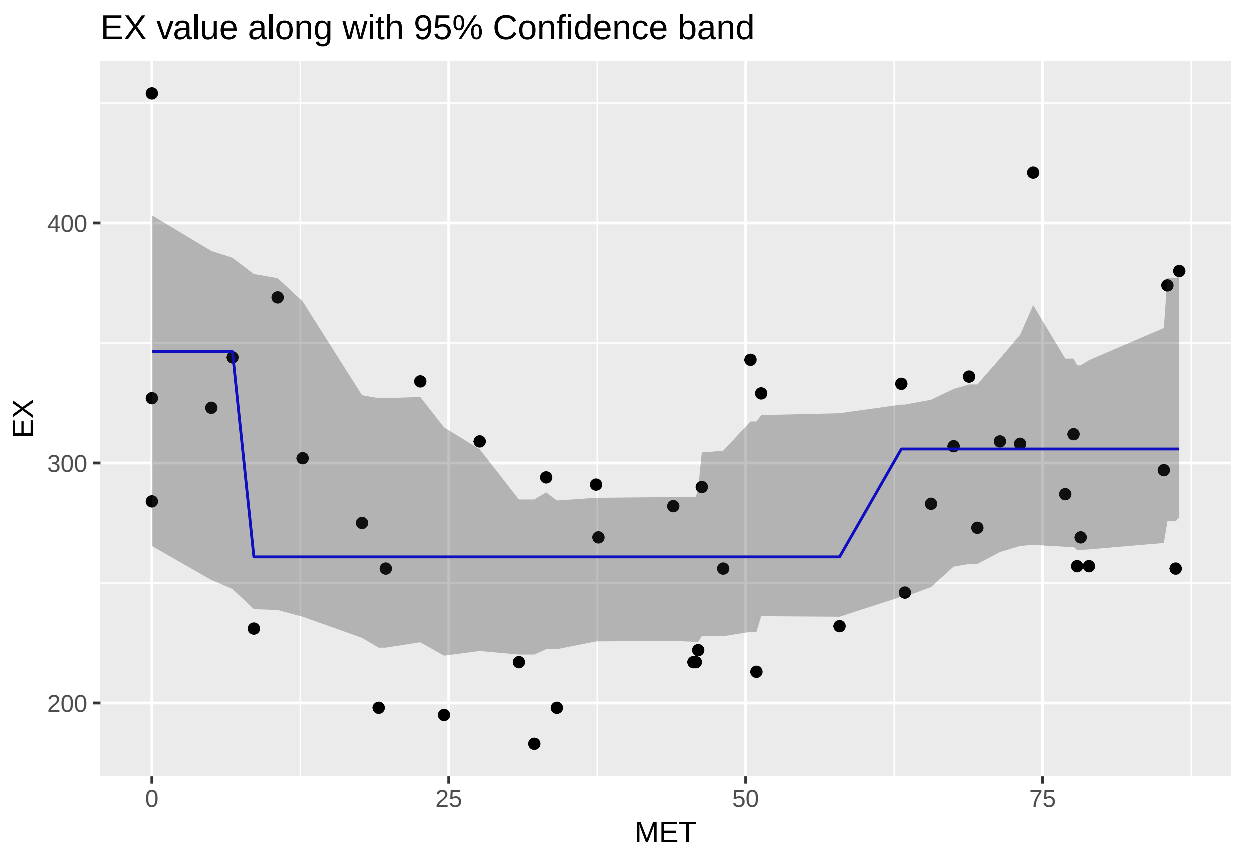
```
## [1] 4663
```

```
out <- p_values[which(p <= 0.05),]
out <- out[order(out$P_value),]
rownames(out) <- NULL
out
```

```
##         feature      P_value
## 1        papers 1.116910e-10
## 2    submission 7.949969e-10
## 3      position 8.219362e-09
## 4     published 1.835157e-07
## 5     important 3.040833e-07
## 6          call 3.983540e-07
## 7    conference 5.091970e-07
## 8    candidates 8.612259e-07
## 9         dates 1.398619e-06
## 10        paper 1.398619e-06
## 11       topics 5.068373e-06
## 12      limited 7.907976e-06
## 13     candidate 1.190607e-05
## 14        camera 2.099119e-05
## 15         ready 2.099119e-05
## 16       authors 2.154461e-05
## 17           phd 3.382671e-05
## 18      projects 3.499123e-05
## 19           org 3.742010e-05
## 20        chairs 5.860175e-05
## 21           due 6.488781e-05
## 22      original 6.488781e-05
## 23  notification 6.882210e-05
## 24        salary 7.971981e-05
## 25        record 9.090038e-05
## 26        skills 9.090038e-05
## 27          held 1.529174e-04
## 28          team 1.757570e-04
## 29         pages 2.007353e-04
## 30      workshop 2.007353e-04
## 31     committee 2.117020e-04
## 32   proceedings 2.117020e-04
## 33         apply 2.166414e-04
## 34        strong 2.246309e-04
## 35 international 2.295684e-04
## 36        degree 3.762328e-04
## 37     excellent 3.762328e-04
## 38          post 3.762328e-04
## 39     presented 3.765147e-04
```

Confidence band using Bootstrap

```
library(boot)
set.seed(12345)
state_data <- read.csv2("state.csv")

# computing bootstrap samples
bootstrap <- function(data, indices){
  data <- state_data[indices,]

  model <- tree(data = data,
       EX~MET,
       control = tree.control(nobs=NROW(data),
                              minsize = 8))

  model_purned <- prune.tree(model, best = 3)
  final_fit_boot <- predict(model_purned, newdata = state_data)
  return(final_fit_boot)
}

res <- boot(state_data, bootstrap, R=1000) #make bootstrap
e <- envelope(res, level = 0.95)
state_tree_regression <- tree(data = state_data, EX~MET,
                              control = tree.control(nobs=NROW(state_data),
                                              minsize = 8))

# puring the tree for leaf size of 3
state_cv_tree_purned <- prune.tree(state_tree_regression, best = 3)
predict_for_ci <- predict(state_cv_tree_purned, state_data)
data_for_ci <- cbind(upper_bound = e$point[1,],
                     lower_bound = e$point[2,],
                     EX = state_data$EX,
                     MET = state_data$MET,
                     predicted_value = predict_for_ci) %>% as.data.frame()

#plot cofidence bands

ggplot(data=data_for_ci, aes(x = MET, y = EX)) +
  geom_point(aes(x = MET,y=EX)) +
  geom_line(aes(x = MET, y=predicted_value), colour="blue") +
  geom_ribbon(aes(x = MET, ymin=lower_bound, ymax=upper_bound),alpha = 0.3) +
  ggtitle("EX value along with 95% Confidence band")
```



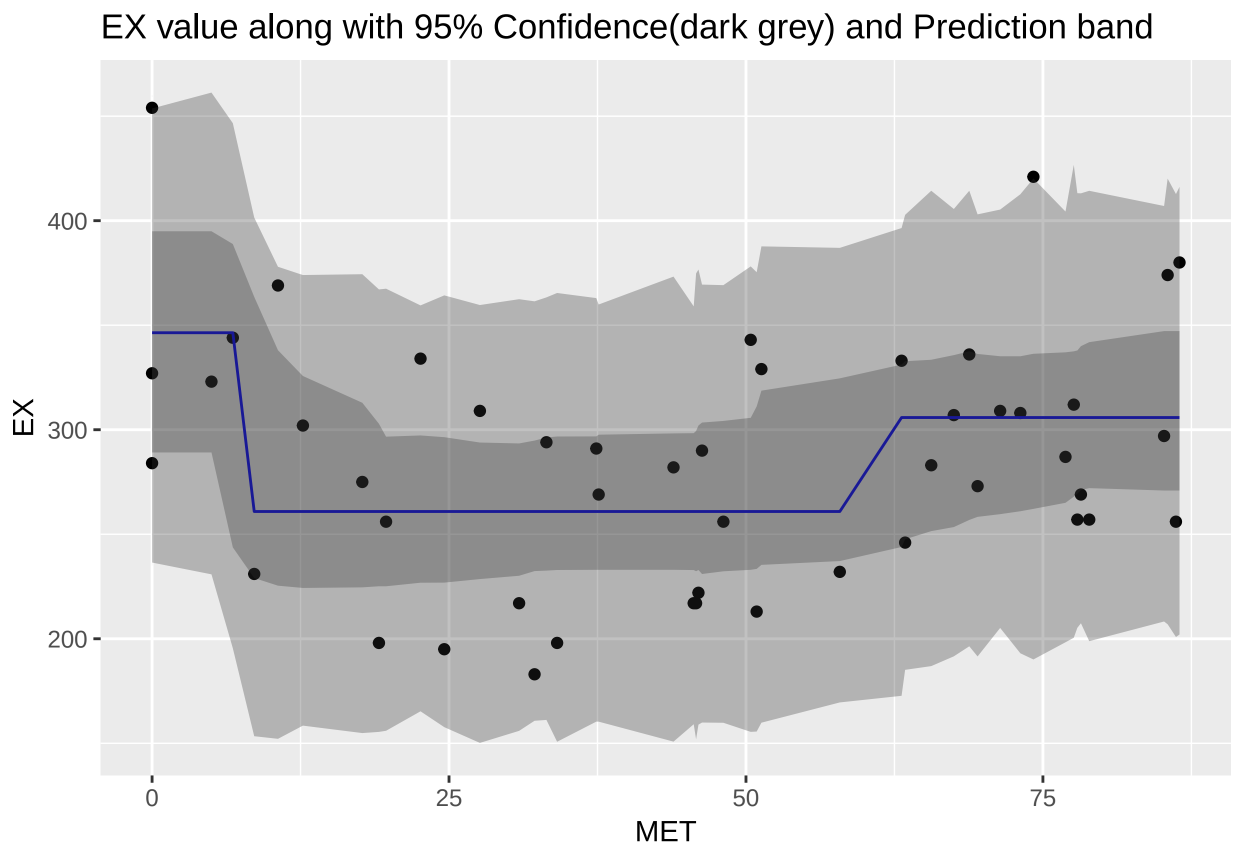
Prediction band using Bootstrap

```
set.seed(12345)
state_tree_regression <- tree(data = state_data, EX~MET,
                              control = tree.control(nobs=NROW(state_data),
                                                              minsize = 8))


mle=prune.tree(state_tree_regression, best = 3)

rng=function(data, mle) {
  data1=data.frame(EX=data$EX, MET=data$MET)
  n=length(data$EX)
  pred <- predict(mle, newdata = data1)
  residual <- data1$EX - pred
#generate new Price
  data1$EX=rnorm(n, pred, sd(residual))
  return(data1)
}

# computing bootstrap samples
conf.fun <- function(data){
  model <- tree(data = data,
       EX~MET,
       control = tree.control(nobs=NROW(data),
                              minsize = 8))

  model_purned <- prune.tree(model, best = 3)
  final_fit_boot <- predict(model_purned, newdata = state_data)
  return(final_fit_boot)
}


# computing bootstrap samples
pred.fun <- function(data){
  model <- tree(data = data,
       EX~MET,
       control = tree.control(nobs=NROW(data),
                              minsize = 8))

  model_purned <- prune.tree(model, best = 3)
  final_fit_boot <- predict(model_purned, newdata = state_data)
  final_fit <- rnorm(n = length(final_fit_boot),  mean = final_fit_boot, sd=sd(residuals(mle)))
  return(final_fit)
}


conf_para = boot(state_data, statistic=conf.fun, R=1000, mle=mle, ran.gen=rng, sim="parametric")
pred_para = boot(state_data, statistic=pred.fun, R=1000, mle=mle, ran.gen=rng, sim="parametric")

e1 <- envelope(conf_para, level = 0.95)
e2 <- envelope(pred_para, level = 0.95)
```

```
## Warning in envelope(pred_para, level = 0.95): unable to achieve requested overall error rate
```

```
# puring the tree for leaf size of 3
state_cv_tree_purned <- prune.tree(state_tree_regression, best = 3)
predict_for_ci <- predict(state_cv_tree_purned, state_data)
```

```r
data_for_ci_para <- cbind(upper_bound = e1$point[1,],
                     lower_bound = e1$point[2,],
                     upper_bound_pred = e2$point[1,],
                     lower_bound_pred = e2$point[2,],
                     EX = state_data$EX,
                     MET = state_data$MET,
                     predicted_value = predict_for_ci) %>% as.data.frame()

ggplot(data=data_for_ci_para, aes(x = MET, y = EX)) +
  geom_point(aes(x = MET,y=EX)) +
  geom_line(aes(x = MET, y=predicted_value), colour="blue") +
  geom_ribbon(aes(x = MET, ymin=lower_bound, ymax=upper_bound),alpha = 0.3) +
  geom_ribbon(aes(x = MET, ymin=lower_bound_pred, ymax=upper_bound_pred), alpha = 0.3) +
  ggtitle("EX value along with 95% Confidence(dark grey) and Prediction band")
```



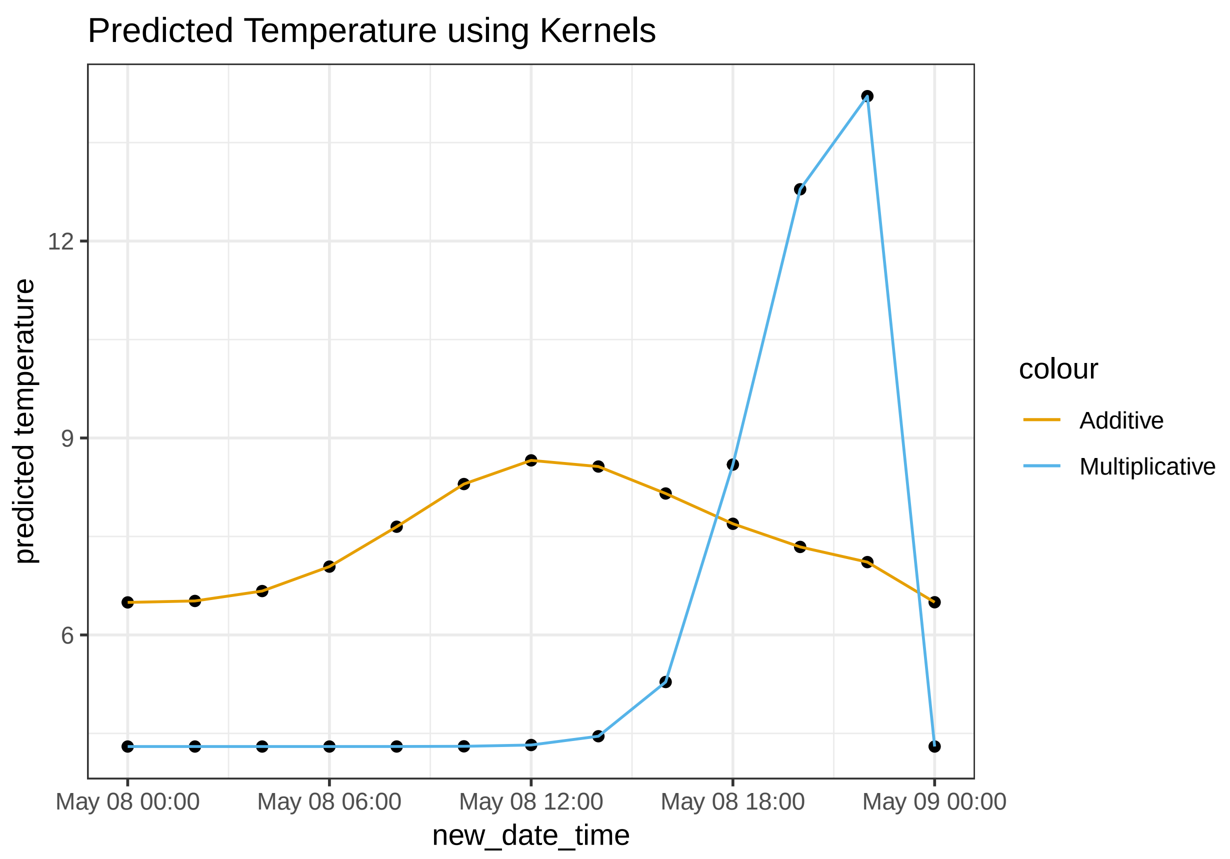
Kernal Estimation

Kernel Smoothing Regression

```r
rm(list=ls())
set.seed(1234567890)
stations <- read.csv("stations.csv")
temps <- read.csv("temps50k.csv")
```

```r
st <- merge(stations,temps,by="station_number")
rm(temps, stations)

st <- st[1:2000,]



kernel_method <- function(df, date, loc_long, loc_lat, h1, h2, h3) {

set.seed(1234567890)
start <- as.POSIXct(date)
interval <- 60
end <- start + as.difftime(1, units="days")
time_seq <- seq(from=start, by=interval*120, to=end)
time_seq <- as.data.frame(time_seq)
colnames(time_seq) <- "new_date_time"
time_seq$time_index <- rownames(time_seq)

df_new <- merge.data.frame(df,time_seq,all=TRUE)
rm(df)

df_new$new_date <- as.Date(df_new$new_date_time)
df_new$new_time <- format(df_new$new_date_time,"%H:%M:%S")
df_new$loc_long <- loc_long
df_new$loc_lat <-  loc_lat


df_new$h_distance <-  abs(geosphere::distHaversine(p1 = df_new[,c("loc_long", "loc_lat")],
                                       p2 = df_new[,c("longitude", "latitude")]))

df_new$h_date <- as.numeric(abs(difftime(df_new$new_date, df_new$date, units = c("days"))))

df_new$h_time <- as.numeric(abs(difftime(strptime(paste(df_new$new_date,
                                                     df_new$new_time),"%Y-%m-%d%H:%M:%S"),
                                        strptime(paste(df_new$new_date, df_new$time),
                                  "%Y-%m-%d %H:%M:%S"),
                         units = c("hour"))))


df_new$date_time <- paste(df_new$date, df_new$time)
df_new$hd_dist <- as.numeric(difftime(df_new$new_date_time,
                         df_new$date_time,
                         units = c("hour")))

## removing any negative dates and time
df_new$posterior_flag <- as.factor(ifelse(df_new$h_distance > 0 & df_new$hd_dist > 0, "retain", "drop")


## calculating kernel distance and choosing guassian kernel
df_new$h_distance_kernel <- exp(-(df_new$h_distance/h1)^2)
df_new$h_date_kernel <- exp(-(df_new$h_date/h2)^2)
df_new$h_time_kernel <- exp(-(df_new$h_time/h3)^2)
df_new$total_additive_dist <- (df_new$h_distance_kernel + df_new$h_date_kernel + df_new$h_time_kernel)
df_new$total_mul_dist <- (df_new$h_distance_kernel * df_new$h_date_kernel * df_new$h_time_kernel)

df_new$additive_num <- ifelse(df_new$posterior_flag == "retain",
                              df_new$h_distance_kernel*df_new$air_temperature +
                                df_new$h_date_kernel*df_new$air_temperature +
                                df_new$h_time_kernel*df_new$air_temperature,0)

df_new$mul_num <- ifelse(df_new$posterior_flag == "retain",
                         (df_new$h_distance_kernel) *
                                (df_new$h_date_kernel) *
                                (df_new$h_time_kernel*df_new$air_temperature),0)

df_new$additive_den <- ifelse(df_new$posterior_flag == "retain", df_new$total_additive_dist, 0)
df_new$mul_den <- ifelse(df_new$posterior_flag == "retain", df_new$total_mul_dist, 0)

time = unique(time_seq$time_index)
result <- NULL

for(i in time){
temp <- df_new[df_new$time_index == i,]
additive_temp <- sum(temp$additive_num)/sum(temp$additive_den)
mult_temp <- sum(temp$mul_num)/sum(temp$mul_den)

temp <- cbind(additive_temp, mult_temp, i)
result <- rbind(temp,result)
}

result <- as.data.frame(result)
result <- merge(x =result, y = time_seq, by.x = "i", by.y = "time_index", all.x = TRUE)
result$additive_temp <- as.numeric(as.character(result$additive_temp))
result$mult_temp <- as.numeric(as.character(result$mult_temp))

p1 <- ggplot(data=result, aes(x=new_date_time)) +
  geom_point(aes(y = additive_temp)) +
  geom_point(aes(y = mult_temp)) +
  geom_line(aes(y = additive_temp, color = "Additive")) +
  geom_line(aes(y = mult_temp, color = "Multiplicative")) +
  scale_color_manual(values=c("#E69F00", "#56B4E9")) +
  ylab("predicted temperature") +
  theme_bw() +
  ggtitle("Predicted Temperature using Kernels")

final <- list(p1)
return(final)
}



kernel_method(df=st, date = "2000-05-08", loc_long = 17.6935,
loc_lat = 59.9953, h1 = 30000, h2 = 2, h3 = 5)
```

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



Onlearning SVM

```
set.seed(1234567890)
spam <- read.csv2("spambase.csv")
ind <- sample(1:nrow(spam))
spam <- spam[ind,c(1:48,58)]
h <- 1
beta <- 0
M <- 50
N <- 500 # number of training points

gaussian_k <- function(x, h) { # It is fine if students use exp(-x**2)/h instead
  return (exp(-(x**2)/(2*h*h)))
}

SVM <- function(sv,i) { #SVM on point i with support vectors sv
  yi <- 0
  for(m in 1:length(sv)) {
    xixm <- rbind(spam[i,-49],spam[sv[m],-49]) # do not use the true label when computing the distance
    tm <- 2 * spam[sv[m],49] - 1 # because the true labels must be -1/+1 and spambase has 0/1
    yi <- yi + tm * gaussian_k(dist(xixm, method="euclidean"), h)
  }
  return (yi)
}
```

```r
errors <- 1
errorrate <- vector(length = N)
errorrate[1] <- 1
sv <- c(1)
for(i in 2:N) {
  yi <- SVM(sv,i)
  ti <- 2 * spam[i,49] - 1

  if(ti * yi < 0) {
    errors <- errors + 1
  }
  errorrate[i] <- errors/i

   cat(".") # iteration ", i, "error rate ", errorrate[i], ti * yi, "sv ", length(sv), "\n")
   flush.console()

  if(ti * yi <= beta) {
    sv <- c(sv, i)

    if (length(sv) > M) {
      for(m in 1:length(sv)) { # remove the support vector that gets classified best without itself
        sv2 <- sv[-m]
        ym2 <- SVM(sv2,sv[m])
        tm <- 2 * spam[sv[m],49] - 1

        if(m==1) {
          max <- tm * ym2
          ind <- 1
        }
        else {
          if(tm * ym2 > max) {
            max <- tm * ym2
            ind <- m
          }
        }
      }
      sv <- sv[-ind]

      # cat("removing ", ind, max, "\n")
      # flush.console()
    }
  }
}
plot(errorrate[seq(from=1, to=N, by=10)], ylim=c(0.2,0.4), type="o")
M
beta
length(sv)
errorrate[N]
```

EM algorithm

Multivariate Gaussian distributions

You are asked to implement the EM algorithm for mixtures of multivariate Gaussian distributions. You should use the following equations in the

E-step:

$$p(z_{nk}|x_n,\mu,\pi) = \frac{\pi_k f(x_n|\mu_k)}{\sum_k \pi_k f(x_n|\mu_k)}$$

M-step:

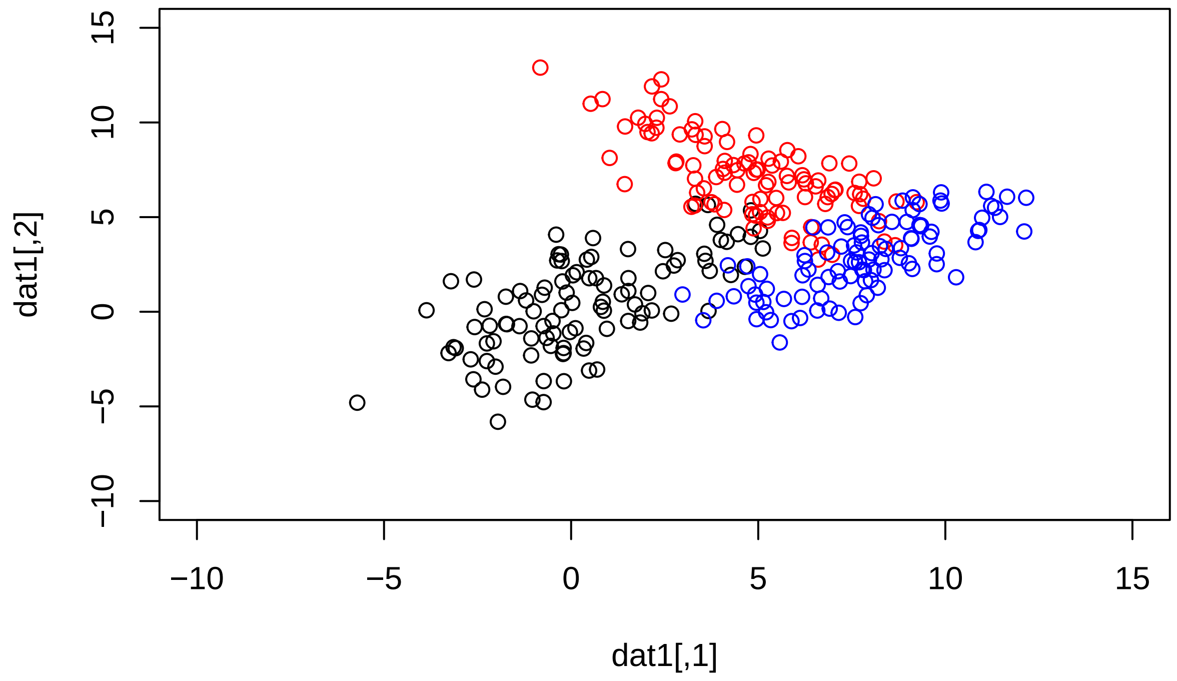
$$\pi_k^{ML} = \frac{\sum_n p(z_{nk}|x_n,\mu,\pi)}{N}$$
$$\mu_k^{ML} = \frac{\sum_n x_n p(z_{nk}|x_n,\mu,\pi)}{\sum_n p(z_{nk}|x_n,\mu,\pi)}$$

$$\sum_k^{ML} = \frac{\sum_n (x_n-\mu_k^{ML})(x_n-\mu_k^{ML})^{ML} p(z_{nk}|x_n,\mu,\pi)}{\sum_n p(z_{nk}|x_n,\mu,\pi)}$$

where f is the density function of a Gaussian distribution, which is implemented by the function dmvnorm in the R package mvtnorm. You can reuse your solution for the corresponding lab assignment. Use the following code for sampling the learning data and initializing the parameters. Note that the learning data consists of 300 points sampled from a mixture model with three equally likely components, and each component is a bivariate Gaussian distribution.

```r
library(mvtnorm)

# Doing as told by the exam instructions.
set.seed(1234567890)

# Max number of EM iterations.
max_it = 100
# min change in log likelihood between two consecutive EM iterations.
min_change = 0.1

# Number of training points.
N = 300

# Number of dimensions.
D = 2

# Training data.
x = matrix(nrow=N, ncol=D)

# Sampling the training data.
# First component.
mu1 = c(0, 0)
Sigma1 = matrix(c(5,3,3,5), D, D)
dat1 = rmvnorm(n=100, mu1, Sigma1)
```

```r
# Second component.
mu2 = c(5, 7)
Sigma2 = matrix(c(5,-3,-3,5), D, D)
dat2 = rmvnorm(n=100, mu2, Sigma2)

# Third component.
mu3 = c(8, 3)
Sigma3 = matrix(c(3,2,2,3), D, D)
dat3 = rmvnorm(n=100, mu3, Sigma3)

# Populating the data set.
x[1:100, ] = dat1
x[101:200, ] = dat2
x[201:300, ] = dat3

true_pi = c(1/3, 1/3, 1/3)

# Plot of the data.
plot(dat1,xlim=c(-10,15),ylim=c(-10,15))
points(dat2,col="red")
points(dat3,col="blue")
```



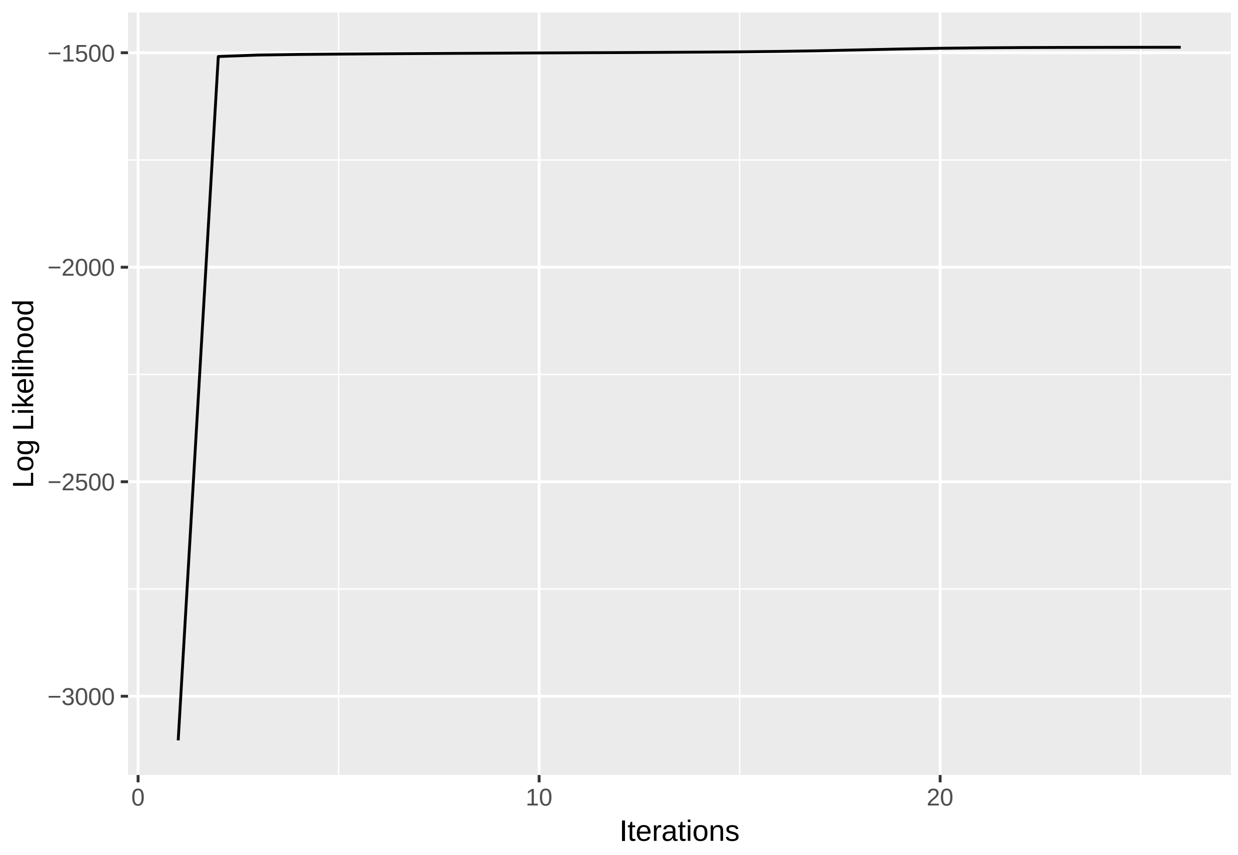
```r
# Initialization of the parameters of the model.
# Number of guessed components.
K = 3
```

```
# Fractional component assignments. AKA latent variable.
z = matrix(nrow=N, ncol=K)

# Mixing coefficients.
pi = vector(length = K)

# Conditional means.
mu = matrix(nrow=K, ncol=D)

# Conditional variances.
Sigma = array(dim=c(D, D, K))

# Variable that stores the log likelihood.
llik = c()

# Random initialization of the parameters.
pi = runif(K, 0, 1)
pi = pi / sum(pi)

for (k in 1:K)
{
 mu[k, ] = runif(D, 0, 5)
 Sigma[, , k] = c(1,0,0,1)
}

get_me_the_F = function(x, mu, Sigma)
{
  mvn_f = matrix(nrow=nrow(x), ncol=3)

  for (i in 1:nrow(x))
  {
    for (j in 1:3)
    {
      mvn_f[i, j] = dmvnorm(x[i, ], mu[j, ], Sigma[ , , j])
    }
  }

  return(mvn_f)
}

######################################
# IMPLEMENTATION OF THE EM ALGORITHM #
######################################

for (i in 1:max_it)
{
  ##########
  # E STEP #
  ##########

  # Multivariate normal density calculation.
  mvn_f = get_me_the_F(x, mu, Sigma)
  # Calculating the posterior.
  numerator_pos = mvn_f * matrix(pi, nrow=nrow(x), ncol=3, byrow=TRUE)
  denominator_pos = rowSums(numerator_pos)
  posterior = numerator_pos / denominator_pos

  ##############################
  # LOOKING IF WE NEED TO STOP #
  ##############################
  llik_i = sum(log(denominator_pos))
  llik = c(llik, llik_i)

  if (i >= 2)
  {
    if (llik[i] - llik[i - 1] < min_change)
    {
      break
    }
  }

  #########
  # M STEP#
  #########

  # Updating pi.
  numerator_pi = colSums(posterior)
  pi = numerator_pi / N

  # Updating mu.
  mu = (t(posterior) %*% x) / numerator_pi

  # Updating each sigma.
  for (k in 1:K)
  {
    shifted_x =(x - matrix(mu[k, ], nrow=N, ncol=2, byrow=TRUE))
    Sigma[ , , k] = (t(shifted_x) %*% (shifted_x * posterior[, k])) / numerator_pi[k]
  }


}
```

plot

Below we can see that the likelihood increases with the number of iterations. We can also see that the parameters are some what close, even though they are not perfectly the same. This might be due to randomness and local optima. Although its pretty clear that the parameters tend to have the same values as the true variables.

```
p = ggplot2::ggplot() +
    ggplot2::geom_line(ggplot2::aes(x=1:length(llik), y=llik)) +
    ggplot2::labs(x="Iterations", y="Log Likelihood")

print(p)
```



```r
# Showing that the true values are close to the estimated.
print("TRUE PI VALUES")
```

```
## [1] "TRUE PI VALUES"
```

```r
print(c(1/3, 1/3, 1/3))
```

```
## [1] 0.3333333 0.3333333 0.3333333
```

```r
print("ESTIMATED PI VALUES")
```

```
## [1] "ESTIMATED PI VALUES"
```

```r
print(pi)
```

```
## [1] 0.2993551 0.3616209 0.3390240
```

```r
print("TRUE MU VALUES")
```

```
## [1] "TRUE MU VALUES"
```

```r
print(mu1)
```

```
## [1] 0 0
```

```r
print(mu2)
```

```
## [1] 5 7
```

```r
print(mu3)
```

```
## [1] 8 3
```

```r
print("ESTIMATED MU VALUES")
```

```
## [1] "ESTIMATED MU VALUES"
```

```r
print(mu)
```

```
##            [,1]       [,2]
## [1,] -0.1096711 -0.0234151
## [2,]  4.9736528  6.8964965
## [3,]  7.5481552  2.8716299
```

```r
print("TRUE SIGMA VALUES")
```

```
## [1] "TRUE SIGMA VALUES"
```

```r
print(Sigma1)
```

```
##      [,1] [,2]
## [1,]    5    3
## [2,]    3    5
```

```r
print(Sigma2)
```

```
##      [,1] [,2]
## [1,]    5   -3
## [2,]   -3    5
```

```r
print(Sigma3)
```

```
##      [,1] [,2]
## [1,]    3    2
## [2,]    2    3
```

```r
print("ESTIMATED SIGMA VALUEs")
```

```
## [1] "ESTIMATED SIGMA VALUEs"
```

```r
print(Sigma)
```

```
## , , 1
##
##          [,1]     [,2]
## [1,] 3.940797 2.706445
## [2,] 2.706445 5.796523
##
## , , 2
##
##           [,1]      [,2]
## [1,]  4.513017 -3.317680
## [2,] -3.317680  5.154163
##
## , , 3
##
##          [,1]     [,2]
## [1,] 4.638160 2.828176
## [2,] 2.828176 3.861886
```

Multivariate Bernoulli distributions

EM is an iterative expectation maximumation technique. The way this works is for a given mixed distribution we guess the components of the data. This is done by first guessing the number of components and then randomly initializing the parameters of the said distribution (Mean, Varience).

Sometimes the data do not follow any known probability distribution but a mixture of known distributions such as:

$$p(x) = \sum_{k=1}^{K} p(k).p(x|k)$$

where p(x|k) are called mixture components and p(k) are called mixing coefficients: where p(k) is denoted by

$$\pi_k$$

With the following conditions

$$0 \leq \pi_k \leq 1$$

and

$$\sum_k \pi_k = 1$$

We are also given that the mixture model follows a Bernoulli distribution, for bernoulli we know that

$$Bern(x|\mu_k) = \prod_i \mu_{ki}^{x_i}.(1-\mu_{ki})^{(1-x_i)}$$

The EM algorithm for an Bernoulli mixed model is:

Set pi and mu to some initial values Repeat until pi and mu do not change E-step: Compute p(z|x) for all k and n M-step: Set pi^k to pi^k(ML) from likehood estimate, do the same to mu

M step:

$$p(z_{nk}|x_n, \mu, \pi) = Z = \frac{\pi_k p(x_n|\mu_k)}{\sum_k p(x_n|\mu_k)}$$

E step:

$$\pi_k^{ML} = \frac{\sum_N p(z_{nk}|x_n, \mu, \pi)}{N}$$

$$\mu_{ki}^{ML} = \frac{\sum_n x_{ni} p(z_{nk}|x_n, \mu, \pi)}{\sum_n p(z_{nk}|x_n, \mu, \pi)}$$

The maximum likehood of E step is:

$$\log_e p(X|\mu, \pi) = \sum_{n=1}^{N} \log_e \sum_{k=1}^{K} .\pi_k.p(x_n|\mu_k)$$

Code

To compare the results for K = 2,3,4, the em_loop-function provides a graphical analysis for every iteration. The function includes comments which explain what I did at which step to create the EM algorithm. The function will be finally run with K = 2,3,4.

```r
em_loop = function(K) {
# Initializing data
set.seed(1234567890)
max_it = 100 # max number of EM iterations
min_change = 0.1 # min change in log likelihood between two consecutive EM iterations
N = 1000 # number of training points
D = 10 # number of dimensions
x = matrix(nrow=N, ncol = D) # training data
true_pi = vector(length = K) # true mixing coefficients
true_mu = matrix(nrow = K, ncol = D) # true conditional distributions
true_pi = c(rep(1/K, K))
if (K == 2) {
true_mu[1,] = c(0.5,0.6,0.4,0.7,0.3,0.8,0.2,0.9,0.1,1)
true_mu[2,] = c(0.5,0.4,0.6,0.3,0.7,0.2,0.8,0.1,0.9,0)
plot(true_mu[1,], type = "o", xlab = "dimension", col = "blue",
ylim = c(0,1), main = "True")
points(true_mu[2,], type="o", xlab = "dimension", col = "red",
main = "True")
} else if (K == 3) {
true_mu[1,] = c(0.5,0.6,0.4,0.7,0.3,0.8,0.2,0.9,0.1,1)
true_mu[2,] = c(0.5,0.4,0.6,0.3,0.7,0.2,0.8,0.1,0.9,0)
true_mu[3,] = c(0.5,0.5,0.5,0.5,0.5,0.5,0.5,0.5,0.5,0.5)
plot(true_mu[1,], type = "o", xlab = "dimension", col = "blue", ylim=c(0,1),
main = "True")
points(true_mu[2,], type = "o", xlab = "dimension", col = "red",
main = "True")
points(true_mu[3,], type = "o", xlab = "dimension", col = "green",
main = "True")
} else {
true_mu[1,] = c(0.5,0.6,0.4,0.7,0.3,0.8,0.2,0.9,0.1,1)
true_mu[2,] = c(0.5,0.4,0.6,0.3,0.7,0.2,0.8,0.1,0.9,0)
true_mu[3,] = c(0.5,0.5,0.5,0.5,0.5,0.5,0.5,0.5,0.5,0.5)
true_mu[4,] = c(0.3,0.5,0.5,0.7,0.5,0.5,0.5,0.5,0.4,0.5)
plot(true_mu[1,], type = "o", xlab = "dimension", col = "blue",
ylim = c(0,1), main = "True")
points(true_mu[2,], type = "o", xlab = "dimension", col = "red",
main = "True")
points(true_mu[3,], type = "o", xlab = "dimension", col = "green",
main = "True")
points(true_mu[4,], type = "o", xlab = "dimension", col = "yellow",
main = "True")
}
z = matrix(nrow = N, ncol = K) # fractional component assignments
pi = vector(length = K) # mixing coefficients
mu = matrix(nrow = K, ncol = D) # conditional distributions
llik = vector(length = max_it) # log likelihood of the EM iterations
# Producing the training data
for(n in 1:N) {
```

```
k = sample(1:K, 1, prob=true_pi)
for(d in 1:D) {
x[n,d] = rbinom(1, 1, true_mu[k,d])
}
}
# Random initialization of the paramters
pi = runif(K, 0.49, 0.51)
pi = pi / sum(pi)
for(k in 1:K) {
mu[k,] = runif(D, 0.49, 0.51)
}
#EM algorithm
for(it in 1:max_it) {
# Plotting mu
# Defining plot title
title = paste0("Iteration", it)
if (K == 2) {
plot(mu[1,], type = "o", xlab = "dimension", col = "blue", ylim = c(0,1), main = title)
points(mu[2,], type = "o", xlab = "dimension", col = "red", main = title)
} else if (K == 3) {
plot(mu[1,], type = "o", xlab = "dimension", col = "blue", ylim = c(0,1), main = title)
points(mu[2,], type = "o", xlab = "dimension", col = "red", main = title)
points(mu[3,], type = "o", xlab = "dimension", col = "green", main = title)
} else {
plot(mu[1,], type = "o", xlab = "dimension", col = "blue", ylim = c(0,1), main = title)
points(mu[2,], type = "o", xlab = "dimension", col = "red", main = title)
points(mu[3,], type = "o", xlab = "dimension", col = "green", main = title)
points(mu[4,], type = "o", xlab = "dimension", col = "yellow", main = title)
}
Sys.sleep(0.5)
# E-step: Computation of the fractional component assignments
for (n in 1:N) {
# Creating empty matrix (column 1:K = p_x_given_k; column K+1 = p(x|all k)
p_x = matrix(data = c(rep(1,K), 0), nrow = 1, ncol = K+1)
# Calculating p(x|k) and p(x|all k)
for (k in 1:K) {
# Calculating p(x|k)
for (d in 1:D) {
p_x[1,k] = p_x[1,k] * (mu[k,d]^x[n,d]) * (1-mu[k,d])^(1-x[n,d])
}
p_x[1,k] = p_x[1,k] * pi[k] # weighting with pi[k]
# Calculating p(x|all k) (denominator)
p_x[1,K+1] = p_x[1,K+1] + p_x[1,k]
}
# Calculating z for n and all k
for (k in 1:K) {
z[n,k] = p_x[1,k] / p_x[1,K+1]
}
}
# Log likelihood computation
for (n in 1:N) {
for (k in 1:K) {
log_term = 0
```

```r
for (d in 1:D) {
log_term = log_term + x[n,d] * log(mu[k,d]) + (1-x[n,d]) * log(1-mu[k,d])
}
llik[it] = llik[it] + z[n,k] * (log(pi[k]) + log_term)
}
}
cat("iteration: ", it, "log likelihood: ", llik[it], "\n")
flush.console()
# Stop if the log likelihood has not changed significantly
if (it != 1) {
if (abs(llik[it] - llik[it-1]) < min_change) {
break
}
}
# M-step: ML parameter estimation from the data and fractional component assignments
# Updating pi
for (k in 1:K) {
pi[k] = sum(z[,k])/N
}
# Updating mu
for (k in 1:K) {
mu[k,] = 0
for (n in 1:N) {
    mu[k,] = mu[k,] + x[n,] * z[n,k]
}
mu[k,] = mu[k,] / sum(z[,k])
}
}
# Printing pi, mu and development of log likelihood at the end
return(list(
pi = pi,
mu = mu,
logLikelihoodDevelopment = plot(llik[1:it],
type = "o",
main = "Development of the log likelihood",
xlab = "iteration",
ylab = "log likelihood")
))
}
```

Running K=2

```r
em_loop(2)
```

Kernel Notes

```r
knitr::include_graphics('./Kernel1.PNG')
```

Kernel Classification

- Consider binary classification with input space $\mathbb{R}^D$.
- The best classifier under the 0-1 loss function is $y^*(\boldsymbol{x}) = \arg\max_y p(y|\boldsymbol{x})$.
- Since $\boldsymbol{x}$ may not appear in the finite training set $\{(\boldsymbol{x}_n, t_n)\}$ available, then classify according to weighted majority voting:

$$y(\boldsymbol{x}) = \begin{cases} 0 & \text{if } \sum_n \mathbf{1}_{\{t_n=1\}} k\left(\frac{\boldsymbol{x}-\boldsymbol{x}_n}{h}\right) \le \sum_n \mathbf{1}_{\{t_n=0\}} k\left(\frac{\boldsymbol{x}-\boldsymbol{x}_n}{h}\right) \\ 1 & \text{otherwise} \end{cases}$$

  where $k : \mathbb{R}^D \to \mathbb{R}$ is a kernel function, which is usually non-negative and monotone decreasing along rays starting from the origin. The parameter h is called smoothing factor or width.

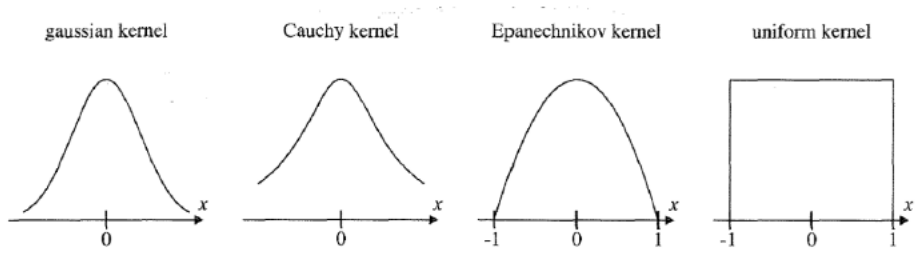
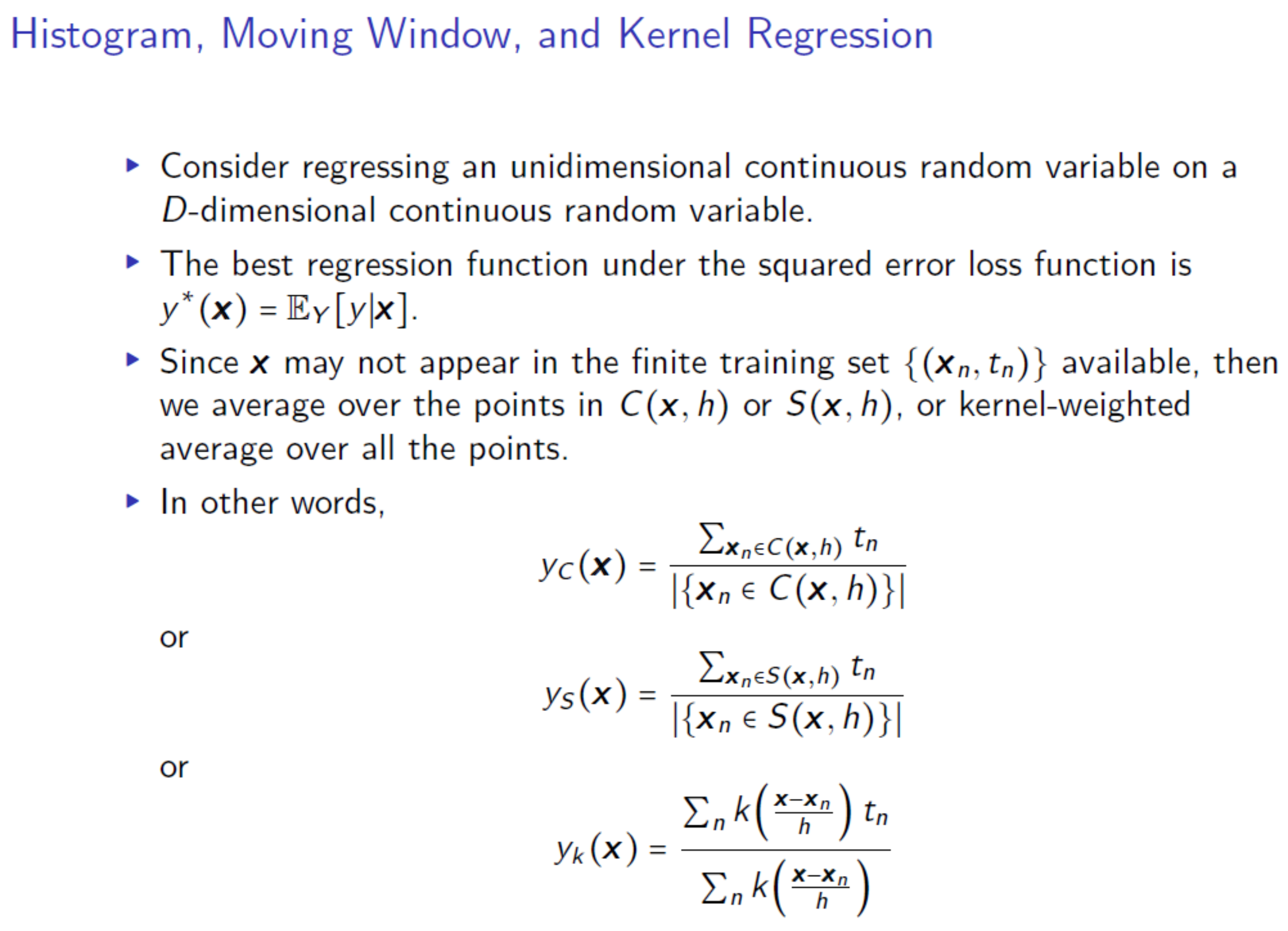


FIGURE 10.3. *Various kernels on $\mathcal{R}$.*

- Gaussian kernel: $k(u) = exp(-||u||^2)$ where $||\cdot||$ is the Euclidean norm.
- Cauchy kernel: $k(u) = 1/(1 + ||u||^{D+1})$
- Epanechnikov kernel: $k(u) = (1 - ||u||^2)\mathbf{1}_{\{||u|| \le 1\}}$

```
knitr::include_graphics('./Kernel2.PNG')
```



Histogram, Moving Window, and Kernel Regression

- Consider regressing an unidimensional continuous random variable on a D-dimensional continuous random variable.
- The best regression function under the squared error loss function is $y^*(\boldsymbol{x}) = \mathbb{E}_Y[y|\boldsymbol{x}]$.
- Since $\boldsymbol{x}$ may not appear in the finite training set $\{(\boldsymbol{x}_n, t_n)\}$ available, then we average over the points in $C(\boldsymbol{x}, h)$ or $S(\boldsymbol{x}, h)$, or kernel-weighted average over all the points.
- In other words,

$$y_C(\boldsymbol{x}) = \frac{\sum_{\boldsymbol{x}_n \in C(\boldsymbol{x},h)} t_n}{|\{\boldsymbol{x}_n \in C(\boldsymbol{x}, h)\}|}$$

or

$$y_S(\boldsymbol{x}) = \frac{\sum_{\boldsymbol{x}_n \in S(\boldsymbol{x},h)} t_n}{|\{\boldsymbol{x}_n \in S(\boldsymbol{x}, h)\}|}$$

or

$$y_k(\boldsymbol{x}) = \frac{\sum_n k\left(\frac{\boldsymbol{x}-\boldsymbol{x}_n}{h}\right) t_n}{\sum_n k\left(\frac{\boldsymbol{x}-\boldsymbol{x}_n}{h}\right)}$$

```r
knitr::include_graphics('./Kernel3.PNG')
```

Histogram, Moving Window, and Kernel Density Estimation

- Consider density estimation for a D-dimensional continuous random variable.
- Let $R \subseteq \mathbb{R}^D$ and $\boldsymbol{x} \in R$. Then,

$$P = \int_R p(\boldsymbol{x}) d\boldsymbol{x} \simeq p(\boldsymbol{x}) Volume(R)$$

  and the number of the N training points $\{\boldsymbol{x}_n\}$ that fall inside R is

$$|\{\boldsymbol{x}_n \in R\}| \simeq P\, N$$

  and thus

$$p(\boldsymbol{x}) \simeq \frac{|\{\boldsymbol{x}_n \in R\}|}{N\, Volume(R)}$$

- Then,

$$p_C(\boldsymbol{x}) = \frac{|\{\boldsymbol{x}_n \in C(\boldsymbol{x}, h)\}|}{N\, Volume(C(\boldsymbol{x}, h))}$$

  or

$$p_S(\boldsymbol{x}) = \frac{|\{\boldsymbol{x}_n \in S(\boldsymbol{x}, h)\}|}{N\, Volume(S(\boldsymbol{x}, h))}$$

  or

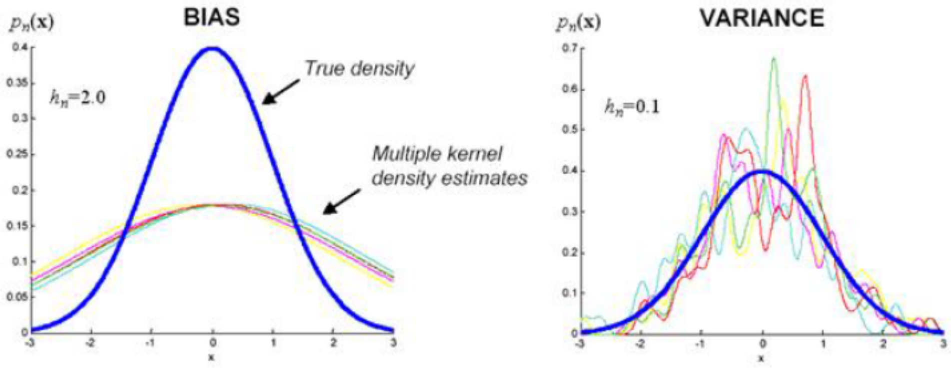
$$p_k(\boldsymbol{x}) = \frac{1}{N} \sum_n k\Big(\frac{\boldsymbol{x} - \boldsymbol{x}_n}{h}\Big)$$

  assuming that $k(u) \geq 0$ for all u and $\int k(u) du = 1$.

```r
knitr::include_graphics('./Kernel4.PNG')
```

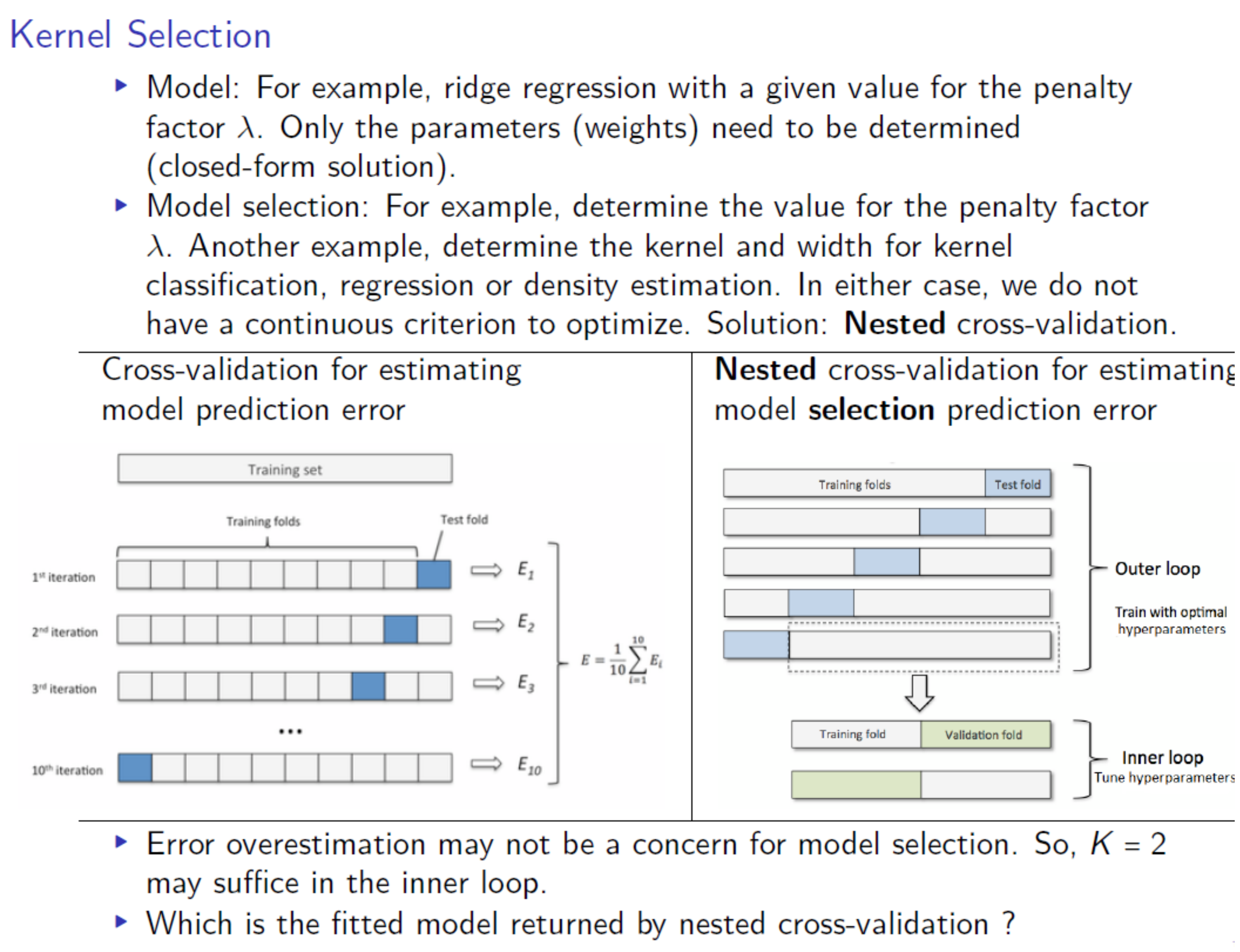
Kernel Selection

- How to choose the right kernel and width ? E.g., by cross-validation.
- What does "right" mean ? E.g., minimize loss function.
- Note that the width of the kernel corresponds to a bias-variance trade-off.



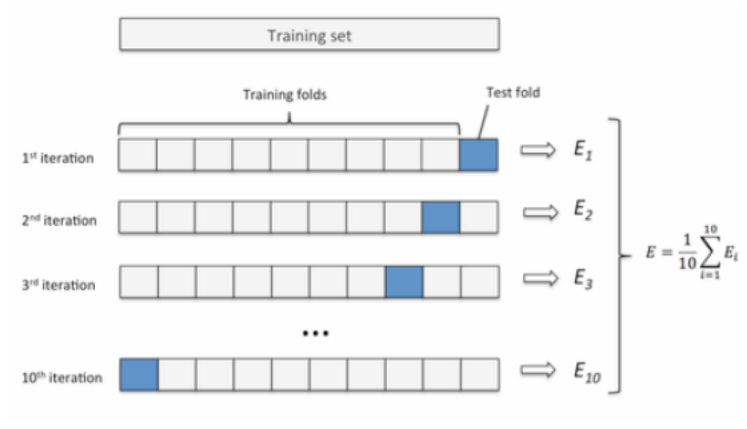
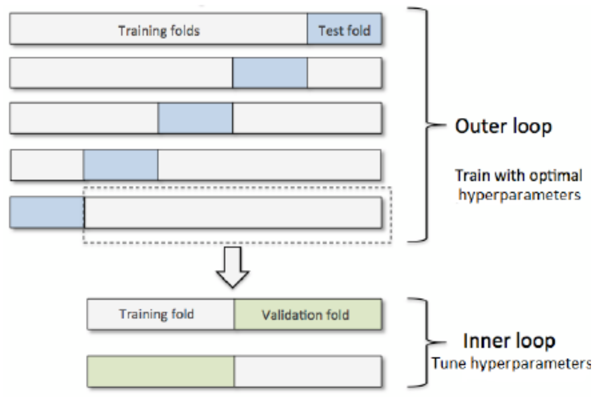
- Small width implies considering few points. So, the variance will be large (similar to the variance of a single point). The bias will be small since the points considered are close to $\boldsymbol{x}$.
- Large width implies considering many points. So, the variance will be small and the bias will be large.

```
knitr::include_graphics('./Kernel5.PNG')
```



Kernel Selection

- Model: For example, ridge regression with a given value for the penalty factor λ. Only the parameters (weights) need to be determined (closed-form solution).
- Model selection: For example, determine the value for the penalty factor λ. Another example, determine the kernel and width for kernel classification, regression or density estimation. In either case, we do not have a continuous criterion to optimize. Solution: **Nested** cross-validation.

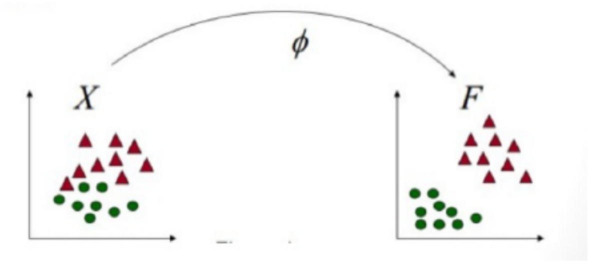
Cross-validation for estimating model prediction error	**Nested** cross-validation for estimating model **selection** prediction error
	

- Error overestimation may not be a concern for model selection. So, $K = 2$ may suffice in the inner loop.
- Which is the fitted model returned by nested cross-validation ?

```
knitr::include_graphics('./Kernel6.PNG')
```

Kernel Trick

- The kernel function $k\left(\frac{x-x'}{h}\right)$ is invariant to translations, and it can be generalized as $k(\boldsymbol{x},\boldsymbol{x}')$. For instance,
  - Polynomial kernel: $k(\boldsymbol{x},\boldsymbol{x}') = (\boldsymbol{x}^T\boldsymbol{x}' + c)^M$
  - Gaussian kernel: $k(\boldsymbol{x},\boldsymbol{x}') = exp(-\|\boldsymbol{x}-\boldsymbol{x}'\|^2/2\sigma^2)$
- If the matrix
$$\begin{pmatrix} k(\boldsymbol{x}_1,\boldsymbol{x}_1) & \dots & k(\boldsymbol{x}_1,\boldsymbol{x}_N) \\ \vdots & \dots & \vdots \\ k(\boldsymbol{x}_N,\boldsymbol{x}_1) & \dots & k(\boldsymbol{x}_N,\boldsymbol{x}_N) \end{pmatrix}$$
is symmetric and positive semi-definite for all choices of $\{\boldsymbol{x}_n\}$, then $k(\boldsymbol{x},\boldsymbol{x}') = \phi(\boldsymbol{x})^T\phi(\boldsymbol{x}')$ where $\phi(\cdot)$ is a mapping from the input space to the feature space.



- The feature space may be non-linear and even infinite dimensional. For instance,
$$\phi(\boldsymbol{x}) = (x_1^2, x_2^2, \sqrt{2}x_1x_2, \sqrt{2c}x_1, \sqrt{2c}x_2, c)$$
for the polynomial kernel with $M = D = 2$.

```r
knitr::include_graphics('./Kernel7.PNG')
```

Kernel Trick

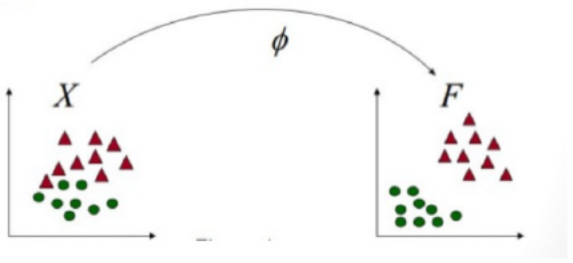
- Consider again moving window classification, regression, and density estimation.
- Note that $\mathbf{x}_n \in S(\mathbf{x}, h)$ if and only if $||\mathbf{x} - \mathbf{x}_n|| \leq h$.
- Note that

$$||\mathbf{x} - \mathbf{x}_n|| = \sqrt{(\mathbf{x} - \mathbf{x}_n)^T(\mathbf{x} - \mathbf{x}_n)} = \sqrt{\mathbf{x}^T\mathbf{x} + \mathbf{x}_n^T\mathbf{x}_n - 2\mathbf{x}^T\mathbf{x}_n}$$

- Then,

$$\begin{aligned} ||\phi(\mathbf{x}) - \phi(\mathbf{x}_n)|| &= \sqrt{\phi(\mathbf{x}^T)\phi(\mathbf{x}) + \phi(\mathbf{x}_n^T)\phi(\mathbf{x}_n) - 2\phi(\mathbf{x}^T)\phi(\mathbf{x}_n)} \\ &= \sqrt{k(\mathbf{x},\mathbf{x}) + k(\mathbf{x}_n,\mathbf{x}_n) - 2k(\mathbf{x},\mathbf{x}_n)} \end{aligned}$$

- So, the distance is now computed in a (hopefully) more convenient space.

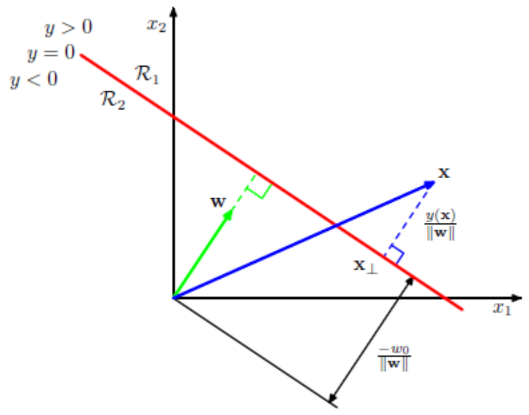


- Note that we do not need to compute $\phi(\mathbf{x})$ and $\phi(\mathbf{x}_n)$.

## SVM Notes

```
knitr::include_graphics('./SVM1.PNG')
```

Support Vector Machines for Classification



- The perpendicular distance from any point to the hyperplane is given by

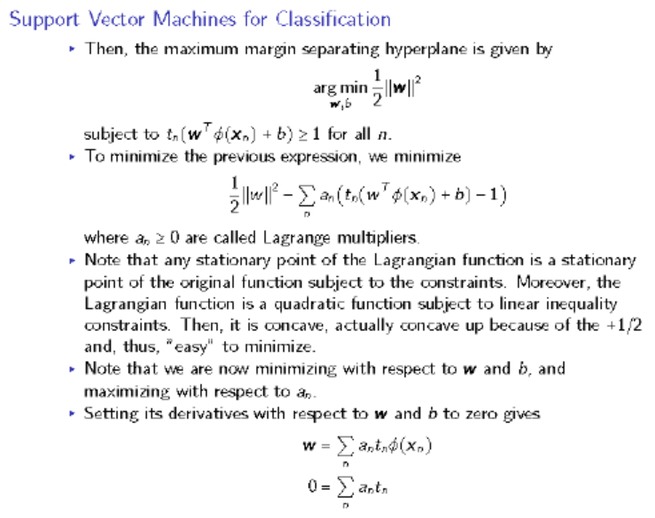
$$\frac{t_n y(\boldsymbol{x}_n)}{||\boldsymbol{w}||} = \frac{t_n(\boldsymbol{w}^T\phi(\boldsymbol{x}_n) + b)}{||\boldsymbol{w}||}$$

- Then, the maximum margin separating hyperplane is given by

$$\arg\max_{\boldsymbol{w},b}\left(\min_n \frac{t_n(\boldsymbol{w}^T\phi(\boldsymbol{x}_n) + b)}{||\boldsymbol{w}||}\right)$$

- Multiply $\boldsymbol{w}$ and b by κ so that $t_n(\boldsymbol{w}^T\phi(\boldsymbol{x}_n) + b) = 1$ for the point closest to the hyperplane. Note that $t_n(\boldsymbol{w}^T\phi(\boldsymbol{x}_n) + b)/||\boldsymbol{w}||$ does not change.

```r
knitr::include_graphics('./SVM2.PNG')
```



Support Vector Machines for Classification

- Then, the maximum margin separating hyperplane is given by

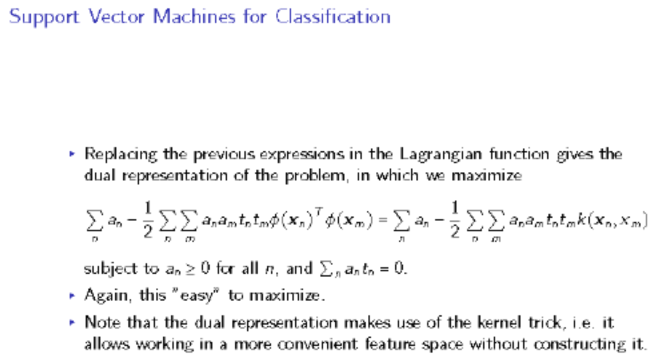
$$\arg\min_{\boldsymbol{w},b} \frac{1}{2}||\boldsymbol{w}||^2$$

  subject to $t_n(\boldsymbol{w}^T\phi(\boldsymbol{x}_n)+b) \geq 1$ for all n.
- To minimize the previous expression, we minimize

$$\frac{1}{2}||w||^2 - \sum_n a_n\big(t_n(w^T\phi(\boldsymbol{x}_n)+b)-1\big)$$

  where $a_n \geq 0$ are called Lagrange multipliers.
- Note that any stationary point of the Lagrangian function is a stationary point of the original function subject to the constraints. Moreover, the Lagrangian function is a quadratic function subject to linear inequality constraints. Then, it is concave, actually concave up because of the +1/2 and, thus, "easy" to minimize.
- Note that we are now minimizing with respect to $\boldsymbol{w}$ and b, and maximizing with respect to a_n.
- Setting its derivatives with respect to $\boldsymbol{w}$ and b to zero gives

$$\boldsymbol{w} = \sum_n a_n t_n \phi(\boldsymbol{x}_n)$$
$$0 = \sum_n a_n t_n$$



Support Vector Machines for Classification

- Replacing the previous expressions in the Lagrangian function gives the dual representation of the problem, in which we maximize

$$\sum_n a_n - \frac{1}{2}\sum_n\sum_m a_n a_m t_n t_m \phi(\boldsymbol{x}_n)^T\phi(\boldsymbol{x}_m) = \sum_n a_n - \frac{1}{2}\sum_n\sum_m a_n a_m t_n t_m k(\boldsymbol{x}_n, x_m)$$

  subject to $a_n \geq 0$ for all n, and $\sum_n a_n t_n = 0$.
- Again, this "easy" to maximize.
- Note that the dual representation makes use of the kernel trick, i.e. it allows working in a more convenient feature space without constructing it.

```r
knitr::include_graphics('./SVM3.PNG')
```

Support Vector Machines for Classification

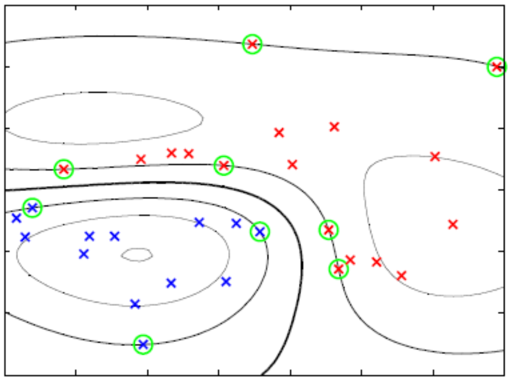
- When the Lagrangian function is maximized, the Karush-Kuhn-Tucker condition holds for all n:

$$a_n(t_n y(\mathbf{x}_n) - 1) = 0$$

- Then, $a_n > 0$ if and only if $t_n y(\mathbf{x}_n) = 1$. The points with $a_n > 0$ are called support vectors and they lie on the margin boundaries.
- A new point $\mathbf{x}$ is classified according to the sign of

$$y(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x}) + b = \sum_n a_n t_n \phi(\mathbf{x}_n)^T \phi(\mathbf{x}) + b = \sum_n a_n t_n k(\mathbf{x}, \mathbf{x}_n) + b$$
$$= \sum_{m \in \mathcal{S}} a_m t_m k(\mathbf{x}, \mathbf{x}_m) + b$$

where $\mathcal{S}$ are the indexes of the support vectors. Sparse solution!



```
knitr::include_graphics('./SVM4.PNG')
```

Support Vector Machines for Classification

- To find b, consider any support vector $\boldsymbol{x}_n$. Then,

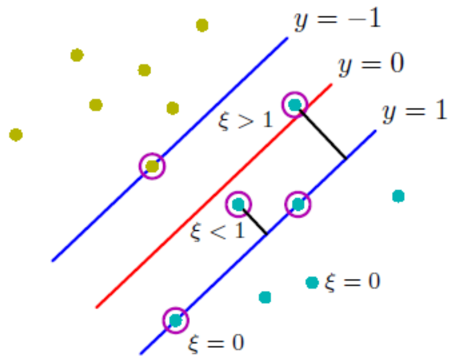
$$1 = t_n y(\boldsymbol{x}_n) = t_n\Big(\sum_{m\in\mathcal{S}} a_m t_m k(\boldsymbol{x}_n, \boldsymbol{x}_m) + b\Big)$$

  and multiplying both sides by t_n, we have that

$$b = t_n - \sum_{m\in\mathcal{S}} a_m t_m k(\boldsymbol{x}_n, \boldsymbol{x}_m)$$

- We now drop the assumption of linear separability in the feature space, e.g. to avoid overfitting. We do so by introducing the slack variables $\xi_n \geq 0$ to penalize (almost-)misclassified points as

$$\xi_n = \begin{cases} 0 & \text{if } t_n y(\boldsymbol{x}_n) \geq 1 \\ |t_n - y(\boldsymbol{x}_n)| & \text{otherwise} \end{cases}$$



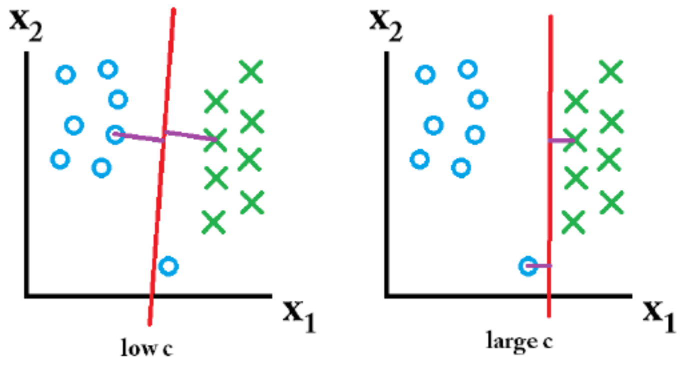
```r
knitr::include_graphics('./SVM5.PNG')
```

Support Vector Machines for Classification

- The optimal separating hyperplane is given by

$$\underset{\boldsymbol{w}, b, \{\xi_n\}}{\arg\min} \frac{1}{2}||\boldsymbol{w}||^2 + C \sum_n \xi_n$$

subject to $t_n y(\boldsymbol{x}_n) \geq 1 - \xi_n$ and $\xi_n \geq 0$ for all n, and where $C > 0$ controls regularization. Its value can be decided by cross-validation. Note that the number of misclassified points is upper bounded by $\sum_n \xi_n$.



- To minimize the previous expression, we minimize

$$\frac{1}{2}||\boldsymbol{w}||^2 + C \sum_n \xi_n - \sum_n a_n \Big(t_n (\boldsymbol{w}^T \phi(\boldsymbol{x}_n) + b) - 1 + \xi_n \Big) - \sum_n \mu_n \xi_n$$

where $a_n \geq 0$ and $\mu_n \geq 0$ are Lagrange multipliers.

```
knitr::include_graphics('./SVM6.PNG')
```

Support Vector Machines for Classification

- Setting its derivatives with respect to $\boldsymbol{w}$, b and ξ_n to zero gives

$$\boldsymbol{w} = \sum_n a_n t_n \phi(\boldsymbol{x}_n)$$
$$0 = \sum_n a_n t_n$$
$$a_n = C - \mu_n$$

- Replacing these in the Lagrangian function gives the dual representation of the problem, in which we maximize

$$\sum_n a_n - \frac{1}{2} \sum_n \sum_m a_n a_m t_n t_m k(\boldsymbol{x}_n, \boldsymbol{x}_m)$$

  subject to $a_n \geq 0$ and $a_n \leq C$ for all n, because $\mu_n \geq 0$.
- When the Lagrangian function is maximized, the Karush-Kuhn-Tucker conditions hold for all n:

$$a_n(t_n y(\boldsymbol{x}_n) - 1 + \xi_n) = 0$$
$$\mu_n \xi_n = 0$$

- Then, $a_n > 0$ if and only if $t_n y(\boldsymbol{x}_n) = 1 - \xi_n$ for all n. The points with $a_n > 0$ are called support vectors and they lie
  - on the margin if $a_n < C$, because then $\mu_n > 0$ and thus $\xi_n = 0$, or
  - inside the margin (even on the wrong side of the decision boundary) if $a_n = C$, because then $\mu_n = 0$ and thus ξ_n is unconstrained.