932A99 - Group K7 - Block 2

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Statement of contribution: Assignment 1 was contributed mostly by Otto, assignment 2 mostly by Ravinder and assignment 3 mostly by Hoda.

1. Assignment 1 - Ensemble methods

This assignment concerns training and analyzing random forests.

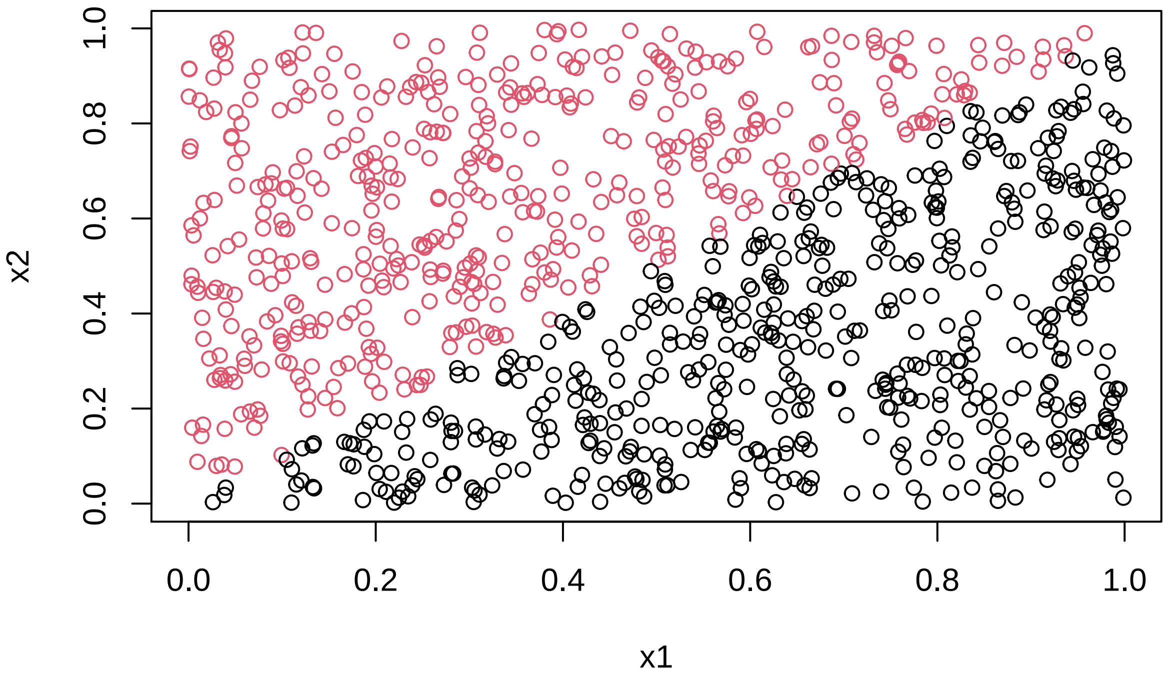
1.1 - Random forest for $y = x1 < x2$

In this section we create 1000 training data sets, each containing 100 observations with three variables. X1 and X2 are generated as random numbers from the uniform distribution with boundaries 0 and 1. Y is then created as a categorical variable based on X1 and X2 with two values; one when X1X2. In total three random forests are learned on each training set, one with 1 tree, one with 10 trees and one with 100 trees. The training data sets are created with the following code:

```
datasets <- list(list(x=0,
                      y=0))
set.seed(12345)
for (set in 1:1000) {
  x1<-runif(100)
  x2<-runif(100)
  trdata<-cbind(x1,x2)
  y<-as.numeric(x1<x2)
  trlabels<-as.factor(y)
  datasets[[set]] <- list(x=trdata,
                      y=trlabels)
}
```

To analyze how these random forests perform a test dataset with 1000 observations is created with the following code:

```
set.seed(1234)
x1<-runif(1000)
x2<-runif(1000)
tedata<-cbind(x1,x2)
y<-as.numeric(x1<x2)
telabels<-as.factor(y)
plot(x1,x2,col=(y+1))
```



With the datasets created the random forests can now be learned with the following code:

```
trees <- c(1,10,100)
forests <- list(list(list()))
set.seed(12345)
for (set in 1:1000) {
  forests[[set]] <- list()
  for (ntrees in 1:3) {
    forests[[set]][[ntrees]] <- randomForest(x = datasets[[set]]$x,
                                             y = datasets[[set]]$y,
                                             xtest = tedata,
                                             ytest = telabels,
                                             ntree = trees[ntrees],
                                             nodesize = 25,
                                             keep.forest = TRUE)
  }
}
```

For these forests the misclassification errors are all calculated. We then compute the mean and variance of this error for all of the random forests with the same amount of trees:

```
# Misclassification  with 1 tree
errors_onetree <- 0
for (set in 1:1000) {
  errors_onetree[set] <- forests[[set]][[1]][["test"]][["err.rate"]][[1]]
}
```

```r
# Misclassification with 10 trees
errors_tentrees <- 0
for (set in 1:1000) {
  errors_tentrees[set] <- forests[[set]][[2]][["test"]][["err.rate"]][[10]]
}

# Misclassification with 100 trees
errors_hundredtrees <- 0
for (set in 1:1000) {
  errors_hundredtrees[set] <- forests[[set]][[3]][["test"]][["err.rate"]][[100]]
}

c(mean(errors_onetree), mean(errors_tentrees), mean(errors_hundredtrees))
```

```
## [1] 0.206499 0.136958 0.113668
```

```r
c(var(errors_onetree), var(errors_tentrees), var(errors_hundredtrees))
```

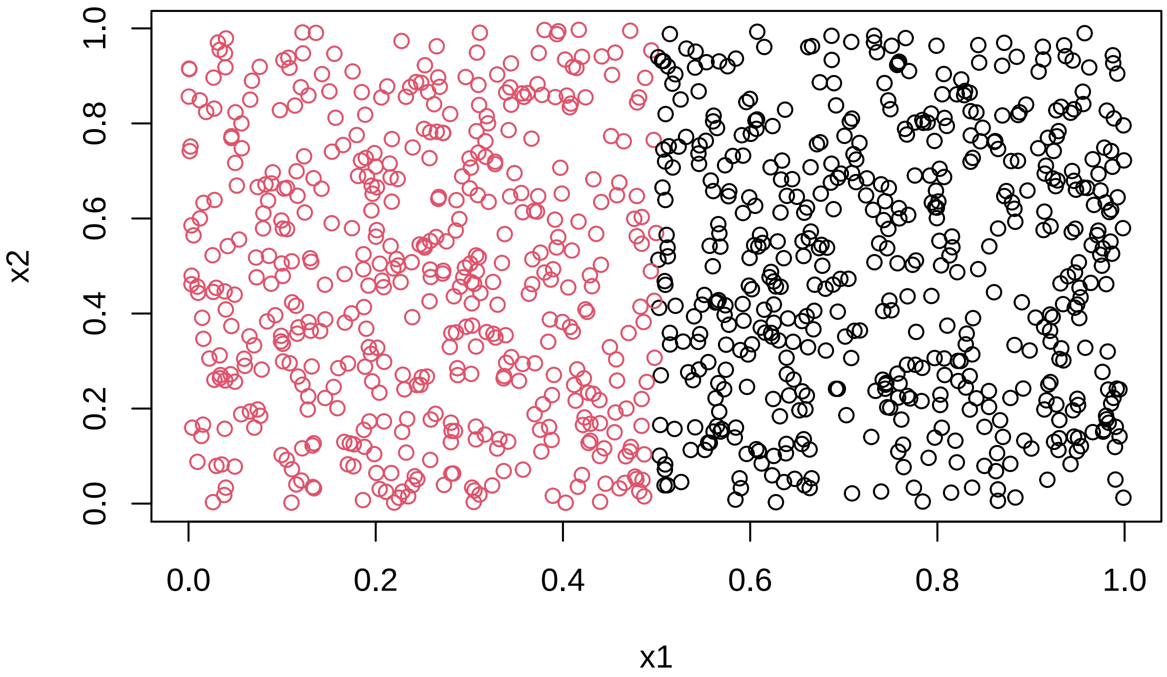
```
## [1] 0.0030611071 0.0010342585 0.0009186224
```

As can be observed the mean misclassification error goes down as the number of trees goes up, from 0.2 at one tree down to 0.11 at one hundred trees. Similarly the variance of the error also goes down as the number of trees goes up.

1.2 - Random forest for y = x1<0.5

In this section we repeat the steps taken in 1.1, but instead compute Y based on X1<0.5 instead. The new data is set up with the following code:

```r
# Generate 1000 data sets
datasets <- list(list(x=0,
                      y=0))
set.seed(12345)
for (set in 1:1000) {
  x1<-runif(100)
  x2<-runif(100)
  trdata<-cbind(x1,x2)
  y<-as.numeric(x1<0.5)
  trlabels<-as.factor(y)

  datasets[[set]] <- list(x=trdata,
                          y=trlabels)
}

# Test data
set.seed(1234)
x1<-runif(1000)
x2<-runif(1000)
tedata<-cbind(x1,x2)
y<-as.numeric(x1<0.5)
telabels<-as.factor(y)
plot(x1,x2,col=(y+1))
```



The random forests are then learned with the following code:

```
trees <- c(1,10,100)
forests_two <- list(list(list()))
set.seed(12345)
for (set in 1:1000) {
  forests_two[[set]] <- list()
  for (ntrees in 1:3) {
    forests_two[[set]][[ntrees]] <- randomForest(x = datasets[[set]]$x,
                                                 y = datasets[[set]]$y,
                                                 xtest = tedata,
                                                 ytest = telabels,
                                                 ntree = trees[ntrees],
                                                 nodesize = 25,
                                                 keep.forest = TRUE)
  }
}
```

Finally the misclassification rates are computed with the following code:

```
# Misclassification  with 1 tree
errors_onetree_two <- 0
for (set in 1:1000) {
  errors_onetree_two[set] <- forests_two[[set]][[1]][["test"]][["err.rate"]][[1]]
}

# Misclassification with 10 trees
```

```r
errors_tentrees_two <- 0
for (set in 1:1000) {
  errors_tentrees_two[set] <- forests_two[[set]][[2]][["test"]][["err.rate"]][[10]]
}

# Misclassification with 100 trees
errors_hundredtrees_two <- 0
for (set in 1:1000) {
  errors_hundredtrees_two[set] <- forests_two[[set]][[3]][["test"]][["err.rate"]][[100]]
}

c(mean(errors_onetree_two), mean(errors_tentrees_two), mean(errors_hundredtrees_two))
```

```
## [1] 0.092144 0.016397 0.007048
```

```r
c(var(errors_onetree_two), var(errors_tentrees_two), var(errors_hundredtrees_two))
```

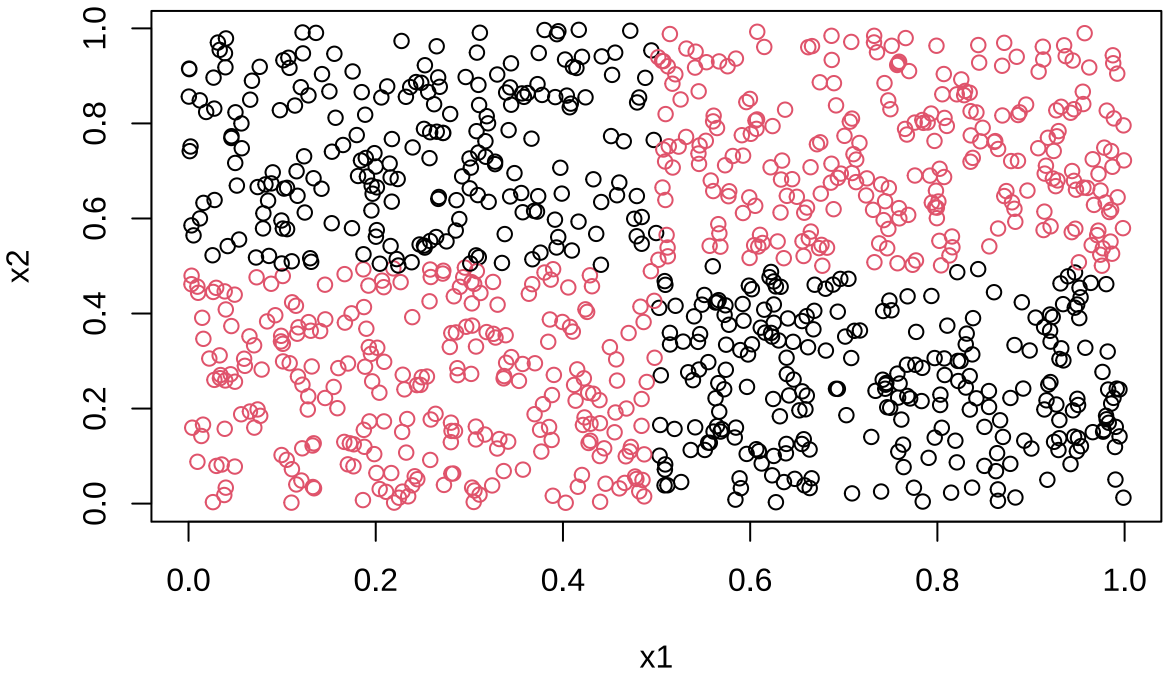
```
## [1] 1.677647e-02 6.196691e-04 9.943113e-05
```

As in the previous section both the mean and variance of the error rate goes down as the number of trees goes up.

1.3 - Random forest for y = x1<05 & x2<0.5 | x1>0.5 & x2>0.5

Once again we repeat the exercise, this time with Y computed based on x1<05 & x2<0.5 or x1>0.5 & x2>0.5. The data is set up with the following code:

```r
# Generate 1000 data sets
datasets <- list(list(x=0,
                      y=0))
set.seed(12345)
for (set in 1:1000) {
  x1<-runif(100)
  x2<-runif(100)
  trdata<-cbind(x1,x2)
  y<-as.numeric((x1<0.5 & x2<0.5)|(x1>0.5 & x2>0.5))
  trlabels<-as.factor(y)

  datasets[[set]] <- list(x=trdata,
                          y=trlabels)
}

set.seed(1234)
x1<-runif(1000)
x2<-runif(1000)
tedata<-cbind(x1,x2)
y<-as.numeric((x1<0.5 & x2<0.5)|(x1>0.5 & x2>0.5))
telabels<-as.factor(y)
plot(x1,x2,col=(y+1))
```



The random forests are then learned with the following code:

```
trees <- c(1,10,100)
forests_three <- list(list(list()))
set.seed(12345)
for (set in 1:1000) {
  forests_three[[set]] <- list()
  for (ntrees in 1:3) {
    forests_three[[set]][[ntrees]] <- randomForest(x = datasets[[set]]$x,
                                                   y = datasets[[set]]$y,
                                                   xtest = tedata,
                                                   ytest = telabels,
                                                   ntree = trees[ntrees],
                                                   nodesize = 12,
                                                   keep.forest = TRUE)
  }
}
```

Finally the misclassification rates are computed with the following code:

```
# Misclassification  with 1 tree
errors_onetree_three <- 0
for (set in 1:1000) {
  errors_onetree_three[set] <- forests_three[[set]][[1]][["test"]][["err.rate"]][[1]]
}

# Misclassification with 10 trees
```

```
errors_tentrees_three <- 0
for (set in 1:1000) {
  errors_tentrees_three[set] <- forests_three[[set]][[2]][["test"]][["err.rate"]][[10]]
}

# Misclassification with 100 trees
errors_hundredtrees_three <- 0
for (set in 1:1000) {
  errors_hundredtrees_three[set] <- forests_three[[set]][[3]][["test"]][["err.rate"]][[100]]
}

c(mean(errors_onetree_three), mean(errors_tentrees_three), mean(errors_hundredtrees_three))
```

```
## [1] 0.250263 0.120546 0.075481
```

```
c(var(errors_onetree_three), var(errors_tentrees_three), var(errors_hundredtrees_three))
```

```
## [1] 0.013511567 0.002977083 0.001216850
```

Just as with the previous two datasets the mean and the variance of the error of the misclassification error goes down as the number of trees goes up.

1.4 - Questions

In this section we answer some questions on the topic of random forests.

a) What happens with the mean and variance of the error rate when the number of trees in the random forest grows?

Overall as the number of trees grows the mean and variance of the error rate goes down.

b) The third dataset represents a slightly more complicated classification problem than the first one. Still, you should get better performance for it when using sufficient trees in the random forest. Explain why you get better performance.

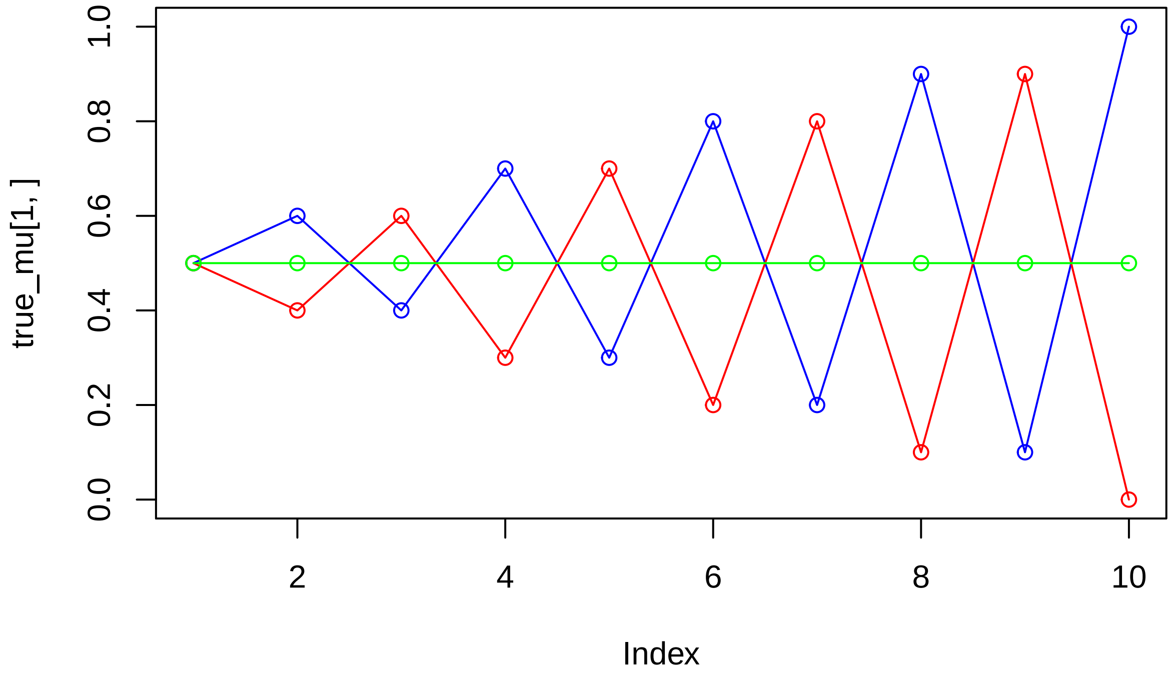
The reason why the performance improves when using more trees is because, even though the problem is a more complicated one, if the trees in general predict better than randomly guessing (error rate of 0.5) then as the number of trees increases they will on average achieve a better result. This is because the final decision for an observation is done by majority voting among the trees in the forest and so if the trees on average do better than random then a larger amount of trees will increase the chance that the majority of them voted for the right class.

c) Why is it desirable to have low error variance?

Low error variance means that a larger amount of the trees in the forest predict correct and incorrect values for the test set at a similar rate. This is desirable as it suggests that the individual trees are not overfitted on their respective training set, which if it were the case would lead to a larger variance as each tree is more dependent on the data it used for training and as such more often return different predictions for the same observation in the test set.

2. Assignment 2 - Mixture model

The problem was to implement expectation minimization algorithm for Bernoulli multivariate mixture model and analyze the estimated parameters and the likelihood for K = 2,3,4.

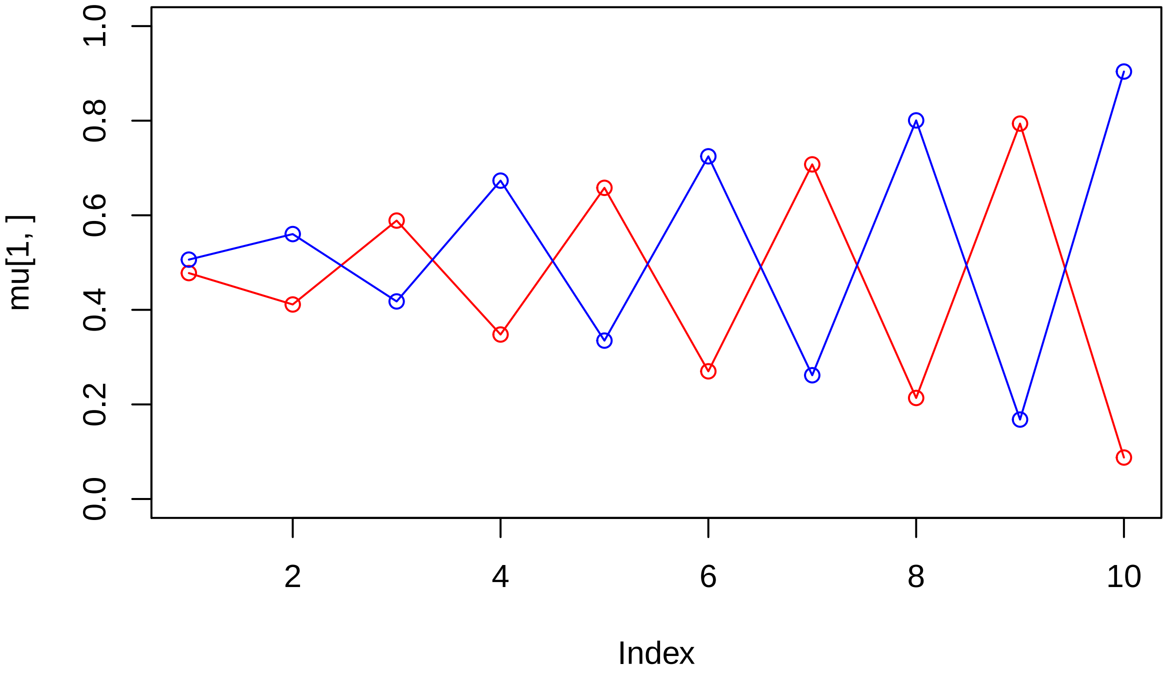


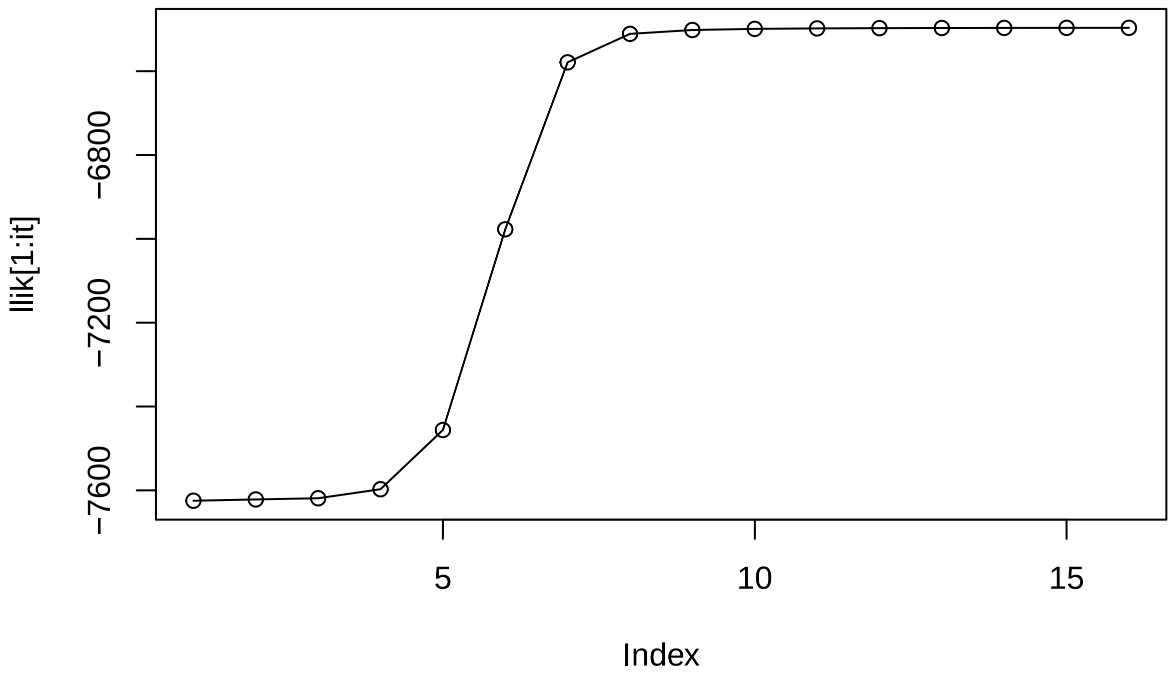
The EM function below takes the number of components(K) as input and prints estimated parameters(pi,mu) and plots mu(for each component) and likelihood over the iterations.

```
EM <- function(k){
  set.seed(1234567890)
  K <- k
  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


  # Random initialization of the parameters
  pi <- runif(K,0.49,0.51)
  pi <- pi / sum(pi)
  for(k in 1:K) {
    mu[k,] <- runif(D,0.49,0.51)
  }

  colors <- c('red','blue','green','yellow')
  for(it in 1:max_it) {

    # E-step: Computation of the fractional component assignments
    for(n in 1:N){
      for(k in 1:K){
        z[n,k] <- pi[k] %*% prod((mu[k,] ^ x[n,]) * ((1-mu[k,]) ^ (1 - x[n,])))
      }
    }
    z <- z / rowSums(z)
    n_k <- colSums(z)
    x_mean_k <- (t(z) %*% x)/n_k


    # Log Likelihood Calculation
    #llik[it] <- sum(t(z) %*% (matrix(log(pi),ncol=K, nrow=N, byrow=TRUE)+
                               #(x %*% t(log(mu)) + (1-x) %*% t(log(1-mu)))))

    llk = 0
    for(i in 1:N){
      for(j in 1:K){
        llk_inner = 0
        for(d in 1:D){
          llk_inner = llk_inner+(x[i,d]*log(mu[j,d])+(1-x[i,d])*log(1-mu[j,d]))
        }
        llk = llk+(z[i,j]) * (log(pi[j])+llk_inner)
      }
    }

    llik[it] = llk

    #cat("iteration: ", it, "log likelihood: ", llik[it], "\n")
    #flush.console()
    # Stop if the log likelihood has not changed significantly
    if(it > 1){
      if((llik[it] - llik[it-1]) <= 0.1){
          break
        }
    }

    #M-step: ML parameter estimation from the data and fractional component assignments

    mu <- x_mean_k
    pi <- n_k/sum(n_k)
  }
  print(pi)
  print(mu)
  plot(mu[1,], type="o", col=colors[1], ylim=c(0,1))
  for(p in 2:K){
    points(mu[p,], type="o",col = colors[p])
  }
  plot(llik[1:it], type="o")
}
```

```
EM(2)
```

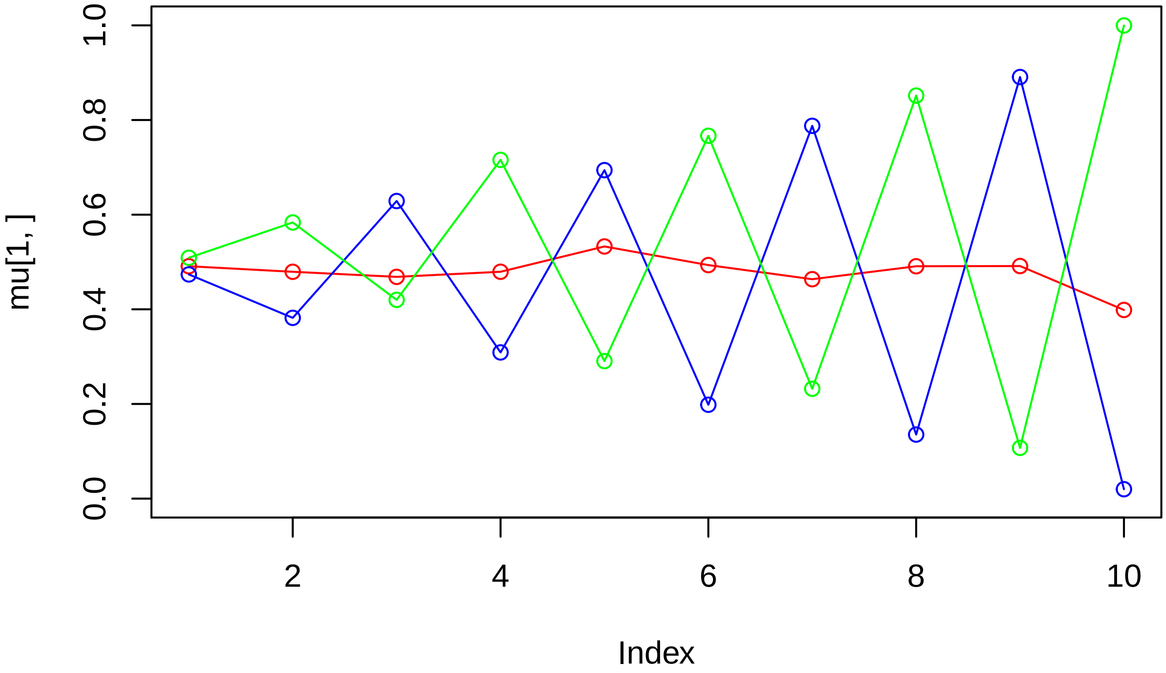
```
## [1] 0.4985208 0.5014792
##           [,1]      [,2]      [,3]      [,4]      [,5]      [,6]      [,7]
## [1,] 0.4777281 0.4113462 0.5887416 0.3477967 0.6580076 0.2700071 0.7076488
## [2,] 0.5061877 0.5602134 0.4177642 0.6732405 0.3349481 0.7246479 0.2616706
##           [,8]      [,9]      [,10]
## [1,] 0.2136319 0.7938673 0.08768382
## [2,] 0.8006315 0.1679843 0.90390147
```

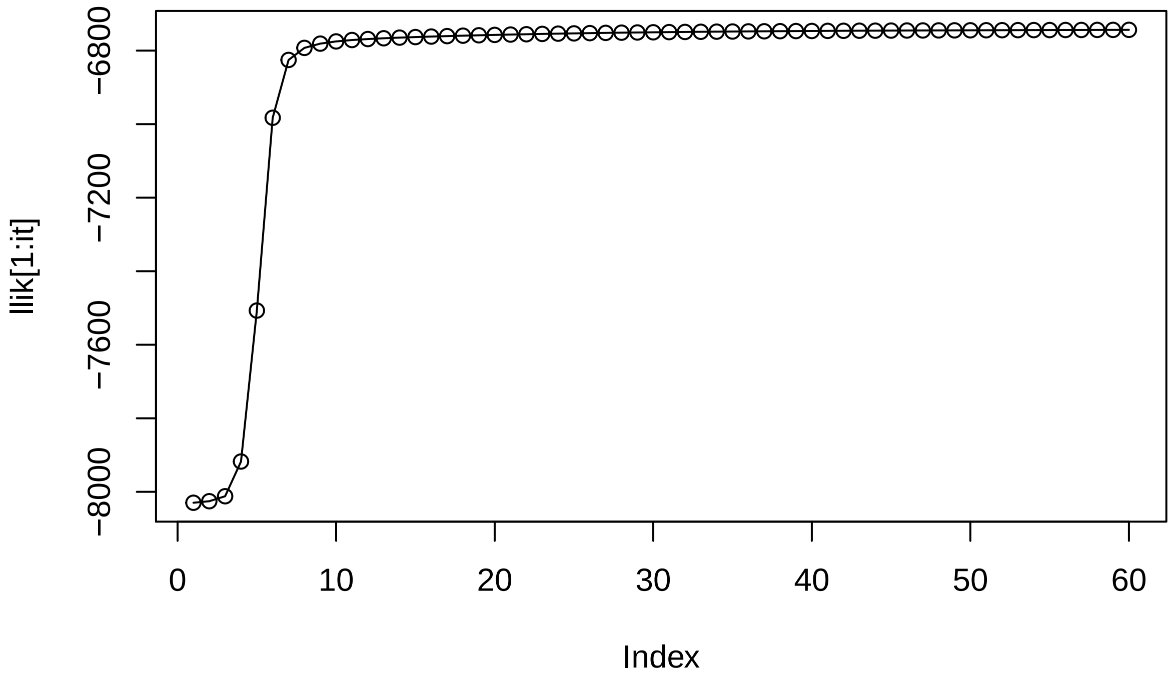




```
EM(3)
```

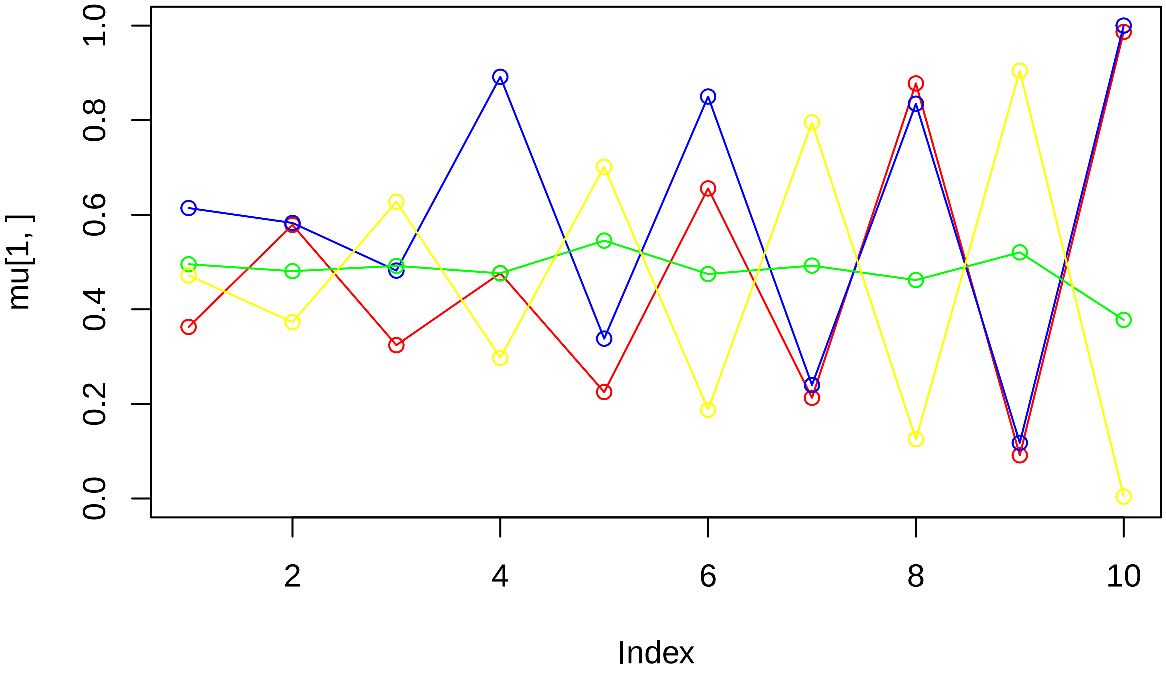
```
## [1] 0.3036757 0.3268051 0.3695192
##           [,1]      [,2]      [,3]      [,4]      [,5]      [,6]      [,7]
## [1,] 0.4910289 0.4792939 0.4686081 0.4793492 0.5328211 0.4934852 0.4636403
## [2,] 0.4737292 0.3819688 0.6287908 0.3089030 0.6941036 0.1983866 0.7876848
## [3,] 0.5089568 0.5835170 0.4200135 0.7157468 0.2905359 0.7666903 0.2321512
##           [,8]      [,9]      [,10]
## [1,] 0.4909945 0.4914184 0.39864411
## [2,] 0.1353086 0.8908487 0.01986696
## [3,] 0.8515860 0.1072591 0.99980959
```

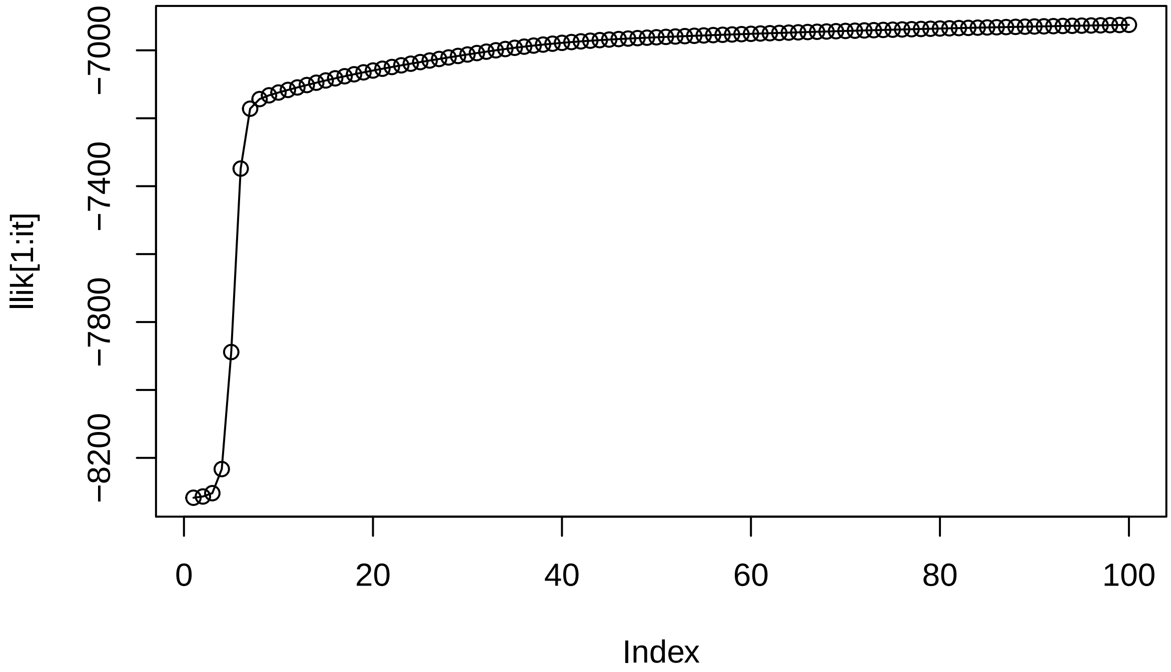

mu[1,]
0.0
0.2
0.4
0.6
0.8
1.0
2
4
6
8
10
Index



```
EM(4)
```

```
## [1] 0.1622641 0.2122779 0.3267767 0.2986813
##           [,1]      [,2]      [,3]      [,4]      [,5]      [,6]      [,7]
## [1,] 0.3628180 0.5784714 0.3242336 0.4764269 0.2250322 0.6557133 0.2129771
## [2,] 0.6142058 0.5826600 0.4819078 0.8916721 0.3380248 0.8500020 0.2400612
## [3,] 0.4953968 0.4807109 0.4918482 0.4761684 0.5453219 0.4746993 0.4924493
## [4,] 0.4716104 0.3728519 0.6273095 0.2973404 0.7015225 0.1876380 0.7953655
##           [,8]       [,9]       [,10]
## [1,] 0.8777434 0.09125969 0.986602810
## [2,] 0.8347953 0.11772402 0.999992227
## [3,] 0.4618857 0.52044305 0.377717125
## [4,] 0.1253232 0.90441870 0.004032343
```


mu[1,]
0.0
0.2
0.4
0.6
0.8
1.0
2
4
6
8
10
Index



Analysis:

K = 2 : As observed when two components were considered likelihood got converged at 16th iteration. Parameter mu for both the components looks similarly distributed.

K = 3 : When three components are used, likelihood took more iterations to converge which approximately around 80. mu for the new component lies between the similar components obtained when two components were used. But,the distance between components 2 and 3 (blue and green to be precise) has increased when compared with plot of 2 components.

K = 4 : Upon using four components, likelihood did converge by the end of 100 iterations. Distribution of mu for the components with blue,green and yellow colors are similar to the one with K=3. The new component with red color line took irregular shape in the start and looked similar towards the end.

3. Assignment 3 - High-dimensional methods

3.1

Dividing the data into training and test sets (70/30) without scaling. Performing nearest shrunken centroid classification of training data in which the threshold is chosen by cross-validation.

```
library(tidyverse)
library(pamr)
library(ggplot2)
library(mgcv)
library(glmnet)
set.seed(12345)
data = read.csv("geneexp.csv")

splitData <- function(data, trainRate) {
  n <- dim(data)[1]
  idxs <- sample(1:n, floor(trainRate*n))
  train <- data[idxs,]
  test <- data[-idxs,]
  return (list(train = train, test = test))
}

split <- splitData(data, 0.7)
train <- split$train
test  <- split$test
y <- train[[ncol(train)]]
x <- t(train[,c(-1,-ncol(train))])
mydata <- list(
  x = x,
  y = as.factor(as.character(y)),
  geneid = as.character(1:nrow(x)),
  genenames = rownames(x)
)

# Training and cross-validating threshold
model <- pamr.train(mydata)
```

```
## 123456789101112131415161718192021222324252627282930
```

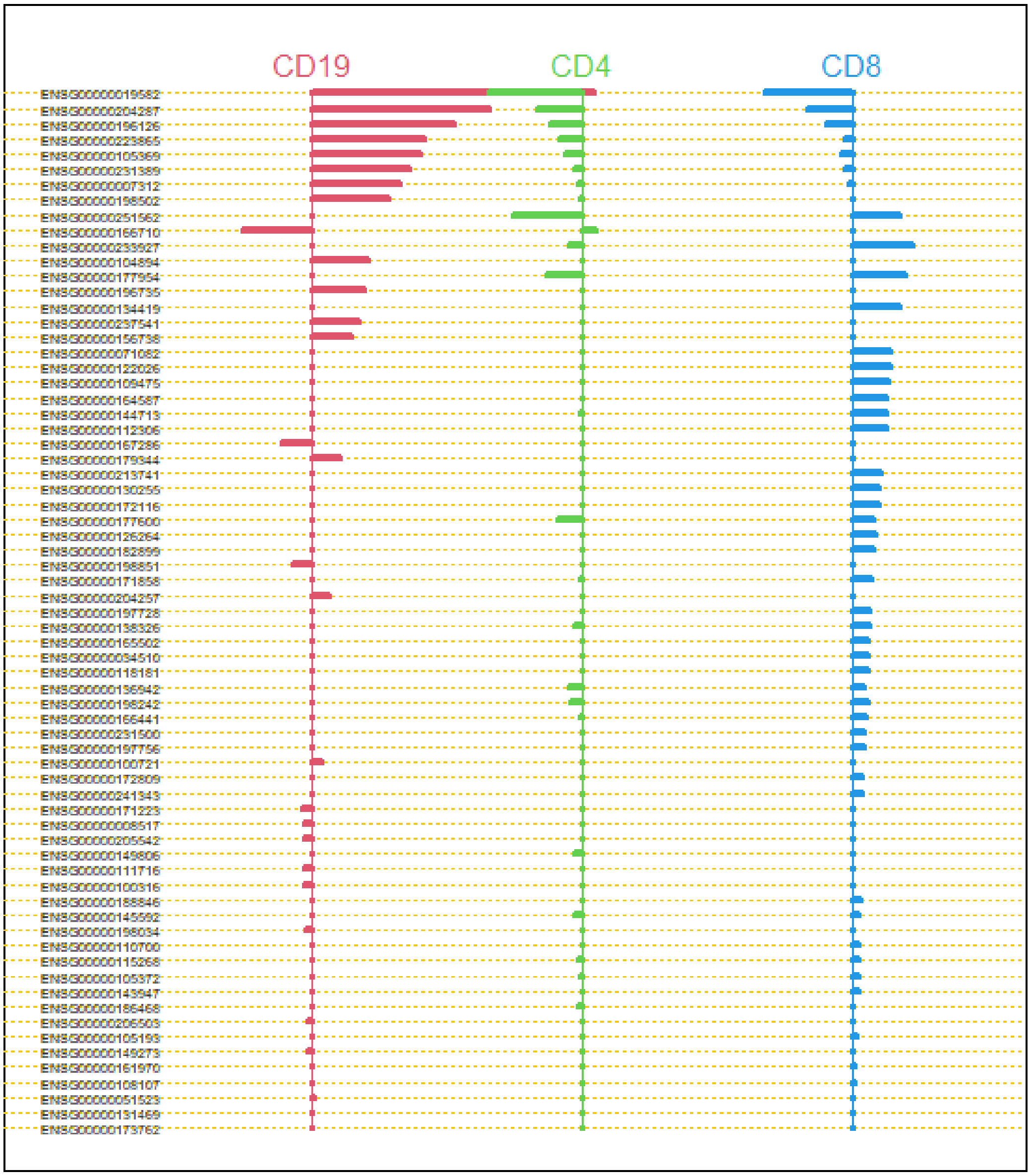
```
cvmodel <- pamr.cv(model, mydata)
```

```
## 123Fold 1 :123456789101112131415161718192021222324252627282930
## Fold 2 :123456789101112131415161718192021222324252627282930
## Fold 3 :123456789101112131415161718192021222324252627282930
## Fold 4 :123456789101112131415161718192021222324252627282930
## Fold 5 :123456789101112131415161718192021222324252627282930
## Fold 6 :123456789101112131415161718192021222324252627282930
## Fold 7 :123456789101112131415161718192021222324252627282930
## Fold 8 :123456789101112131415161718192021222324252627282930
## Fold 9 :123456789101112131415161718192021222324252627282930
## Fold 10 :123456789101112131415161718192021222324252627282930
```

the central plot of genes:

```
## 1
```

```
##       id  name            CD19-score CD4-score CD8-score
##  [1,] 2   ENSG00000019582 1.5153     -0.4617   -0.4489
##  [2,] 15  ENSG00000204287 0.7328     -0.0448   -0.032
##  [3,] 31  ENSG00000196126 0.6715     -0.0105   -0.001
##  [4,] 32  ENSG00000223865 0.5403     0         0
##  [5,] 37  ENSG00000231389 0.4089     0         0
##  [6,] 138 ENSG00000105369 0.4019     0         0
##  [7,] 1   ENSG00000251562 0          -0.3933   0.2553
##  [8,] 90  ENSG00000198502 0.3727     0         0
##  [9,] 172 ENSG00000007312 0.3016     0         0
## [10,] 126 ENSG00000104894 0.2974     0         0
## [11,] 79  ENSG00000233927 0          0         0.2028
## [12,] 11  ENSG00000177954 0          -0.1239   0.1074
## [13,] 110 ENSG00000196735 0.1109     0         0
## [14,] 21  ENSG00000164587 0          0         0.1078
## [15,] 3   ENSG00000166710 -0.1057    0         0
## [16,] 50  ENSG00000071082 0          0         0.1051
## [17,] 207 ENSG00000167286 -0.0933    0         0
## [18,] 29  ENSG00000122026 0          0         0.0914
## [19,] 192 ENSG00000237541 0.0862     0         0
## [20,] 309 ENSG00000156738 0.0438     0         0
## [21,] 28  ENSG00000177600 0          -0.0426   0
## [22,] 38  ENSG00000134419 0          0         0.0346
## [23,] 18  ENSG00000144713 0          0         0.0189
## [24,] 127 ENSG00000213741 0          0         0.0156
## [25,] 36  ENSG00000109475 0          0         0.0119
```



centroid plot shows the distance from the selected gene mean value to the global mean value. positive means that the gene is greater than global mean and negative means that the gene is smaller than the global mean value as a result they can not all be positive for some gene.

```
cat("the number of selected genes is:",length(unique(selectedGenes[,2])))
```

```
## the number of selected genes is: 25
```

the plot of the missclassification error:

```
#grDevices::dev.new()
pamr.plotcv(cvmodel)
```

```
print(cvmodel)
```

```
## Call:
## pamr.cv(fit = model, data = mydata)
##    threshold nonzero errors
## 1   0.000    2058    24
## 2   0.801    1040    22
## 3   1.603     374    25
## 4   2.404     226    25
## 5   3.206     147    25
## 6   4.007     102    23
## 7   4.809      78    24
## 8   5.610      54    23
## 9   6.412      35    25
## 10  7.213      25    21
## 11  8.014      19    22
## 12  8.816      11    21
## 13  9.617      10    26
## 14 10.419       8    39
## 15 11.220       7    70
## 16 12.022       4    72
## 17 12.823       4    73
## 18 13.624       3    73
## 19 14.426       2    73
## 20 15.227       1    73
## 21 16.029       1    73
## 22 16.830       1    72
## 23 17.632       1    72
## 24 18.433       1    72
## 25 19.235       1    72
## 26 20.036       1    71
## 27 20.837       1    70
## 28 21.639       1    70
## 29 22.440       1    92
## 30 23.242       0    118
```

```
best_threshold = cvmodel$threshold[which.min(cvmodel$error)]
bestModel <- pamr.train(mydata, threshold = best_threshold)
```

```
## 1
```

```
#grDevices::dev.new()
```

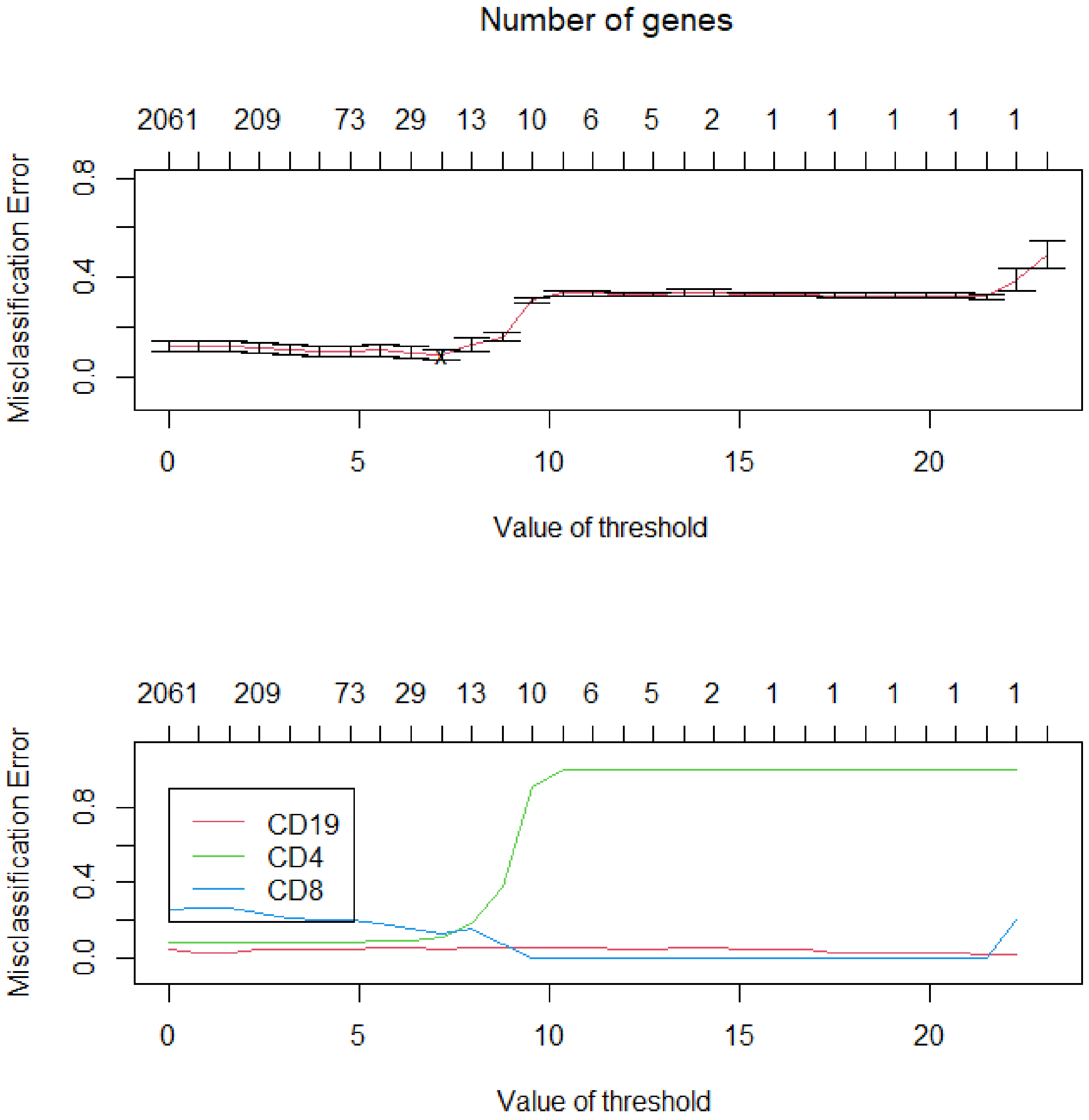


Figure 1: miss-classification Error

```
cat("the best threshod is: ", best_threshold)
```

```
## the best threshod is:  7.212944
```

3.2

```
yTest <- test[[ncol(test)]]
xTest <- t(test[,c(-1,-ncol(test))])
predictions <- pamr.predict(bestModel, newx = xTest, type = "class",
                                threshold = best_threshold)
table(predictions,yTest)
```

```
##            yTest
## predictions CD19 CD4 CD8
##        CD19   27   0   0
##        CD4     0  26   6
##        CD8     0   4  27
```

```
tt <-selectedGenes[,2]
cat("2 most repeated genes:",tt[1],tt[2],"\n")
```

```
## 2 most repeated genes: ENSG00000019582 ENSG00000204287
```

```
cat("the name ENSG00000204287 Gene is  HLA-DRA and this gene is a marker. ","\n")
```

```
## the name ENSG00000204287 Gene is  HLA-DRA and this gene is a marker.
```

```
cat("The name of ENSG00000019582 Gene is CD74 and this gene is a marker.")
```

```
## The name of ENSG00000019582 Gene is CD74 and this gene is a marker.
```

```
cat("test error for NSC : ",1-sum(diag(table(yTest,predictions)))/length(predictions))
```

```
## test error for NSC :  0.1111111
```

3.3.a

Computing the test error and the number of the contributing features for the following methods fitted to the training data: Elastic net with the binomial response and $\alpha = 0.5$ in which penalty is selected by the cross-validation:

```
cvElastNet <- cv.glmnet(x=t(x), y=y, alpha=0.5, type.measure = "mse",family="multinomial")
grDevices::dev.new()
plot(cvElastNet)
optLamdba <- cvElastNet$lambda.min
print("optimal lambda:")
```

```
## [1] "optimal lambda:"
```

```
optLamdba
```

```
## [1] 0.008238962
```

```
elasticnetModel <- glmnet(x = t(x), y = y, family="multinomial",
                          alpha=0.5, lambda = optLamdba)
predictionsElast <- predict(elasticnetModel, newx = t(xTest), type="class")
table(yTest, predictionsElast)
```

```
##       predictionsElast
## yTest  CD19 CD4 CD8
##   CD19   27   0   0
##   CD4     0  29   1
##   CD8     1   3  29
```

```
cat("test error: ",1-sum(diag(table(predictionsElast,yTest)))/length(predictionsElast))
```

```
## test error:  0.05555556
```

```
coeffs <- coef(elasticnetModel)
nonzeroCoeffsCD19 <- coeffs[which(coeffs$CD19 != 0)]
selectedCoeffsCD19 <- length(nonzeroCoeffsCD19)

nonzeroCoeffsCD4 <- coeffs[which(coeffs$CD4 != 0)]
selectedCoeffsCD4 <- length(nonzeroCoeffsCD4)

nonzeroCoeffsCD8 <- coeffs[which(coeffs$CD8 != 0)]
selectedCoeffsCD8 <- length(nonzeroCoeffsCD8 )

cat("Elasticnet model has ", selectedCoeffsCD4, " nonzero coefficients for CD4\n")
```

```
## Elasticnet model has  76  nonzero coefficients for CD4
```

```
cat("Elasticnet model has ", selectedCoeffsCD19, " nonzero coefficients for CD19\n")
```

```
## Elasticnet model has  32  nonzero coefficients for CD19
```

```
cat("Elasticnet model has ", selectedCoeffsCD8, " nonzero coefficients for CD8\n")
```

```
## Elasticnet model has  55  nonzero coefficients for CD8
```

3.3.b

```
library(kernlab)
library(dplyr)
library(tidyr)
data <-  read.csv("geneexp.csv")

names(train)[ncol(train)] <- "Celltype"
train$Celltype <- as.factor(train$Celltype)
for (i in 2:2086) {
  train[,i] <- as.numeric(train[,i])
}

svmModel <- ksvm(Celltype ~., data=train[,-1], kernel="vanilladot", scaled=FALSE)
```

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

```
svmPredictions <- predict(svmModel, test)

cat("SVM table \n")
```

```
## SVM table
```

```
print(table(yTest,svmPredictions))
```

```
##       svmPredictions
## yTest  CD19 CD4 CD8
##   CD19   27   0   0
##   CD4     0  30   0
##   CD8     0   2  31
```

```
cat("\n test error for SVM: ",1-sum(diag(table(yTest,svmPredictions)))/length(svmPredictions))
```

```
##
##  test error for SVM:  0.02222222
```

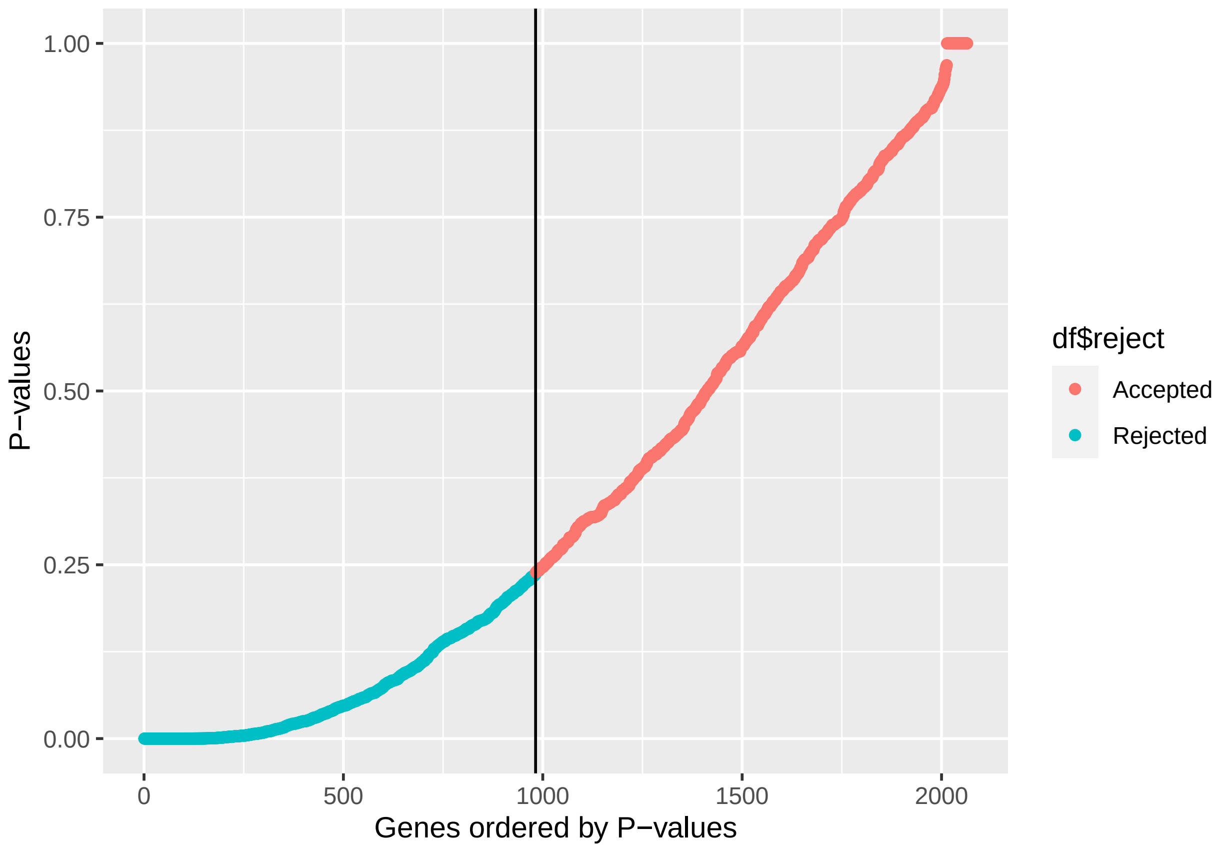
The test error for SVM is the lower than NSC and Elastic net with Cross Validation, as a result we chose SVM.

Modal	MSE
NSC	0.1
Elastic net	0.05
SVM	0.01

3.4

for this task we implement Benjamini-Hochberg method for the original data in which we tested each cell type versus the remaining ones. Here, False discovery rate (FDR) is the expected proportion of tests which are incorrectly called significant out of all the tests which are called significant. We used a larger Value for FDR (0.5) due the nature of our data set. and The Benjamini-Hochberg (BH) method is a procedure which controls the false discovery rate so that FDR <= α.

```
data = read.csv("geneexp.csv")
y <- as.factor(data[,ncol(data)])
data <- as.matrix(data[,c(-1,-ncol(data))])
# Remove variables that only contain 0
data <- data[,-c(43,
                 69,
                 179,
                 188,
                 217,
                 384,
                 527,
                 540,
                 600,
                 647,
                 1044,
                 1146,
                 1330,
                 1370,
                 1435,
                 1505,
                 1900,
                 1944,
                 1972,
                 1983,
                 2027)]


y1 <- as.factor(as.numeric(y=="CD4"))

pvals1 <- as.numeric(vector(length = ncol(data)))
df <- data.frame(
  word = colnames(data),
  pvals <- pvals1
)
BH1 <- as.numeric(vector(length =ncol(data)))

FDR <- 0.5
CL  <- 0.95



for(i in 1:length(pvals1)) {
  test <- t.test(data[,i]~y1,
                 alternative = "two.sided",
                 conf.level = CL )
  df[i,2] <- test$p.value
  BH1[i] <- (FDR * i / length(pvals1))
}

# order increasingly the pvalues
df <- df[order(df$pvals, decreasing = FALSE),]
df <- cbind(df, BH1)
L <- max(which(df[,2] < df[,3]))
df$reject <- c(rep("Rejected",L), rep("Accepted",(2064-L)))


ggplot() +
  geom_point(aes(x=1:nrow(df), y=df[,2], color=df$reject)) +
  geom_vline(xintercept = L)+
  xlab("Genes ordered by P-values") +
  ylab("P-values")
```

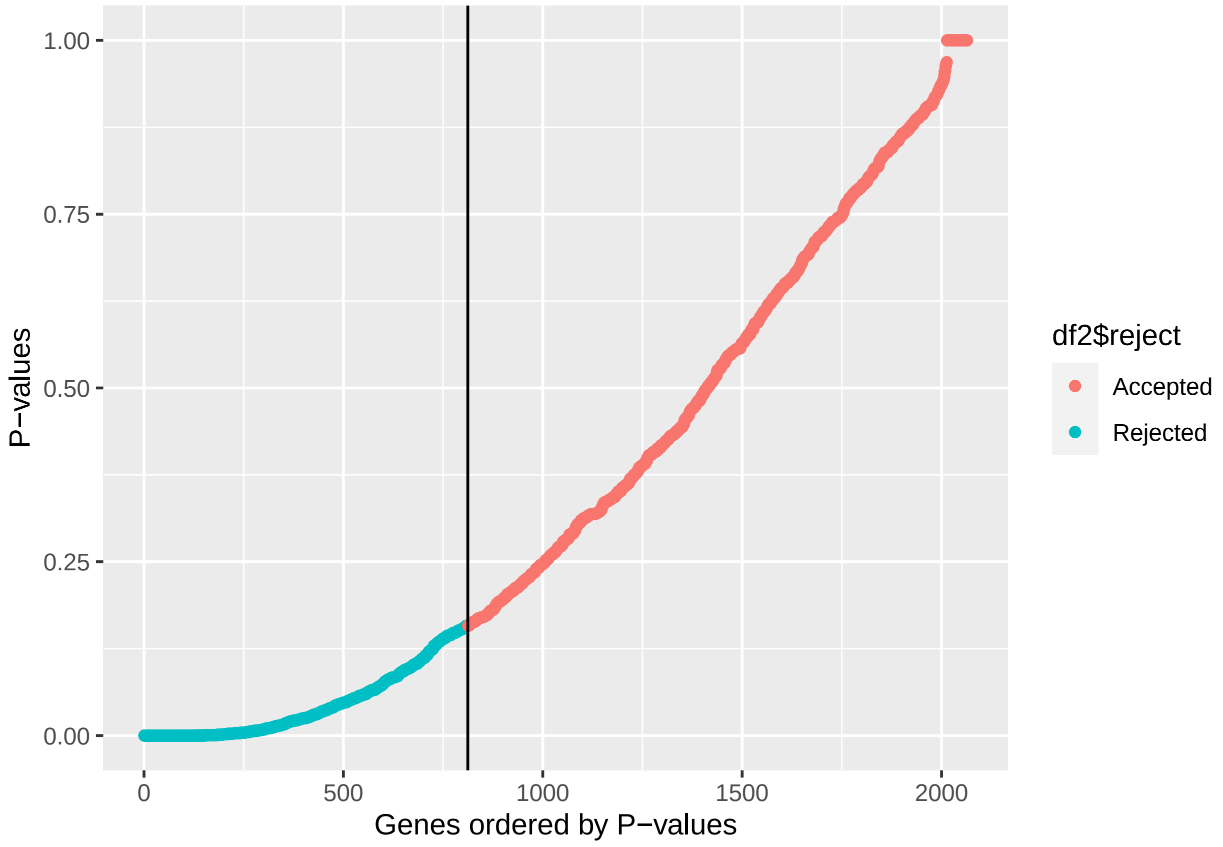


```
cat("Number of Rejected Features CD4 =", L, "\n")
```

```
## Number of Rejected Features CD4 = 982
```

```
y2 <- as.factor(as.numeric(y=="CD8"))

pvals2 <- as.numeric(vector(length = ncol(data)))
df2 <- data.frame(
  word = colnames(data),
  pvals <- pvals2
)
BH2 <- as.numeric(vector(length =ncol(data)))

FDR <- 0.5
CL  <- 0.95



for(i in 1:length(pvals2)) {
  test <- t.test(data[,i]~y2,
               alternative = "two.sided",
               conf.level = CL )
  df2[i,2] <- test$p.value
  BH2[i] <- (FDR * i / length(pvals2))
}
```

```
# order increasingly the pvalues
df2 <- df2[order(df2$pvals, decreasing = FALSE),]
df2 <- cbind(df2, BH2)
L2 <- max(which(df2[,2] < df2[,3]))
df2$reject <- c(rep("Rejected",L2), rep("Accepted",(2064-L2)))


ggplot() +
  geom_point(aes(x=1:nrow(df2), y=df[,2], color=df2$reject)) +
  geom_vline(xintercept = L2)+
  xlab("Genes ordered by P-values") +
  ylab("P-values")
```

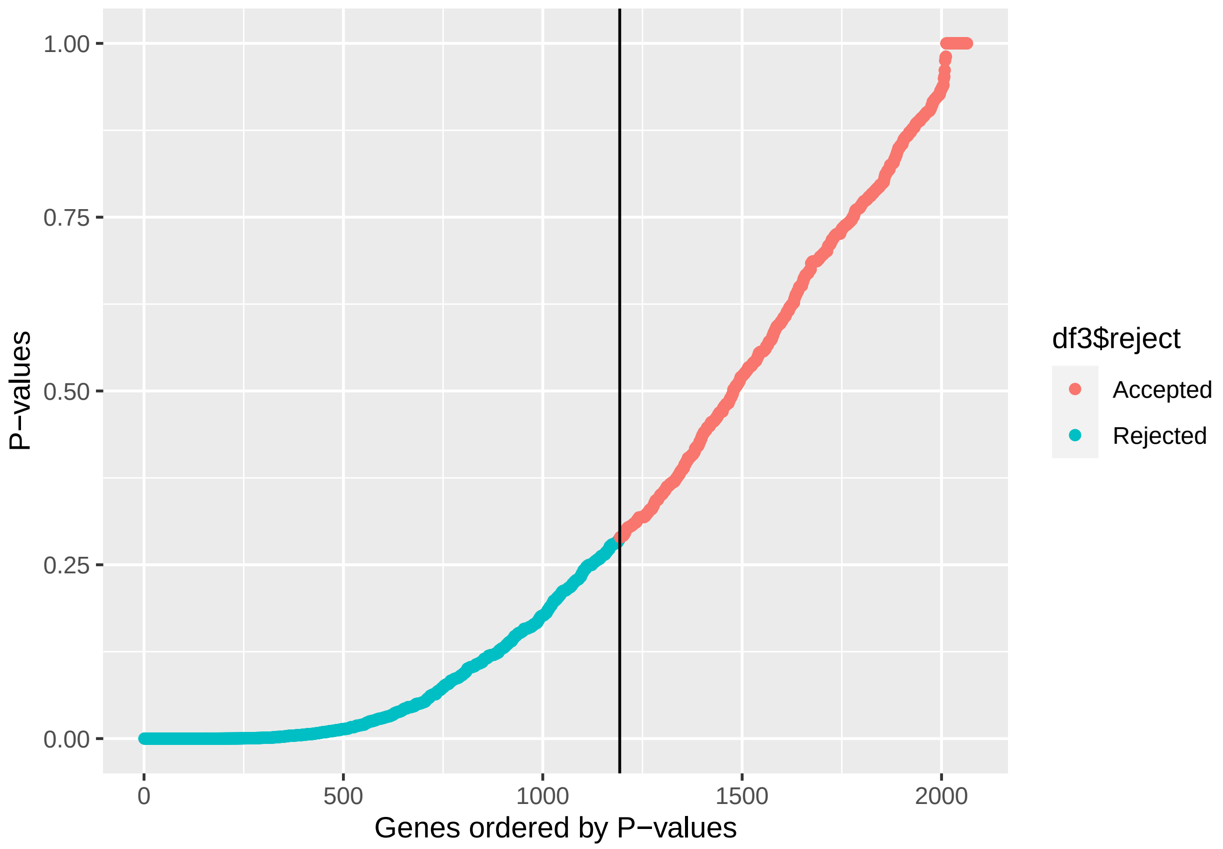


```
cat("Number of Rejected Features CD8: ", L2, "\n" )
```

```
## Number of Rejected Features CD8:  812
```

```
y3 <- as.factor(as.numeric(y=="CD19"))

pvals3 <- as.numeric(vector(length = ncol(data)))
df3 <- data.frame(
  word = colnames(data),
  pvals <- pvals3
)
```

```r
BH3 <- as.numeric(vector(length =ncol(data)))

FDR <- 0.5
CL  <- 0.95



for(i in 1:length(pvals3)) {
  test <- t.test(data[,i]~y3,
                 alternative = "two.sided",
                 conf.level = CL )
  df3[i,2] <- test$p.value
  BH3[i] <- (FDR * i / length(pvals3))
}

# order increasingly the pvalues
df3 <- df3[order(df3$pvals, decreasing = FALSE),]
df3 <- cbind(df3, BH3)
L3 <- max(which(df3[,2] < df3[,3]))
df3$reject <- c(rep("Rejected",L3), rep("Accepted",(2064-L3)))


ggplot() +
  geom_point(aes(x=1:nrow(df3), y=df3[,2], color=df3$reject)) +
  geom_vline(xintercept = L3)+
  xlab("Genes ordered by P-values") +
  ylab("P-values")
```



```
cat("Number of Rejected Features CD19: ", L3 ,"\n")
```

```
## Number of Rejected Features CD19:  1193
```

Appendix: Assignment Code

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

## 1.1
datasets <- list(list(x=0,
                      y=0))
set.seed(12345)
for (set in 1:1000) {
  x1<-runif(100)
  x2<-runif(100)
  trdata<-cbind(x1,x2)
  y<-as.numeric(x1<x2)
  trlabels<-as.factor(y)
  datasets[[set]] <- list(x=trdata,
                      y=trlabels)
}

set.seed(1234)
x1<-runif(1000)
x2<-runif(1000)
tedata<-cbind(x1,x2)
y<-as.numeric(x1<x2)
telabels<-as.factor(y)
plot(x1,x2,col=(y+1))


trees <- c(1,10,100)
forests <- list(list(list()))
set.seed(12345)
for (set in 1:1000) {
  forests[[set]] <- list()
  for (ntrees in 1:3) {
    forests[[set]][[ntrees]] <- randomForest(x = datasets[[set]]$x,
                                             y = datasets[[set]]$y,
                                             xtest = tedata,
                                             ytest = telabels,
                                             ntree = trees[ntrees],
                                             nodesize = 25,
                                             keep.forest = TRUE)
  }
}

# Misclassification  with 1 tree
errors_onetree <- 0
for (set in 1:1000) {
  errors_onetree[set] <- forests[[set]][[1]][["test"]][["err.rate"]][[1]]
}

# Misclassification with 10 trees
errors_tentrees <- 0
```

```r
for (set in 1:1000) {
  errors_tentrees[set] <- forests[[set]][[2]][["test"]][["err.rate"]][[10]]
}

# Misclassification with 100 trees
errors_hundredtrees <- 0
for (set in 1:1000) {
  errors_hundredtrees[set] <- forests[[set]][[3]][["test"]][["err.rate"]][[100]]
}

c(mean(errors_onetree), mean(errors_tentrees), mean(errors_hundredtrees))
c(var(errors_onetree), var(errors_tentrees), var(errors_hundredtrees))

## 1.2
# Generate 1000 data sets
datasets <- list(list(x=0,
                      y=0))
set.seed(12345)
for (set in 1:1000) {
  x1<-runif(100)
  x2<-runif(100)
  trdata<-cbind(x1,x2)
  y<-as.numeric(x1<0.5)
  trlabels<-as.factor(y)

  datasets[[set]] <- list(x=trdata,
                      y=trlabels)
}

# Test data
set.seed(1234)
x1<-runif(1000)
x2<-runif(1000)
tedata<-cbind(x1,x2)
y<-as.numeric(x1<0.5)
telabels<-as.factor(y)
plot(x1,x2,col=(y+1))

trees <- c(1,10,100)
forests_two <- list(list(list()))
set.seed(12345)
for (set in 1:1000) {
  forests_two[[set]] <- list()
  for (ntrees in 1:3) {
    forests_two[[set]][[ntrees]] <- randomForest(x = datasets[[set]]$x,
                                             y = datasets[[set]]$y,
                                             xtest = tedata,
                                             ytest = telabels,
                                             ntree = trees[ntrees],
                                             nodesize = 25,
                                             keep.forest = TRUE)
  }
}
```

```r
# Misclassification  with 1 tree
errors_onetree_two <- 0
for (set in 1:1000) {
  errors_onetree_two[set] <- forests_two[[set]][[1]][["test"]][["err.rate"]][[1]]
}

# Misclassification with 10 trees
errors_tentrees_two <- 0
for (set in 1:1000) {
  errors_tentrees_two[set] <- forests_two[[set]][[2]][["test"]][["err.rate"]][[10]]
}

# Misclassification with 100 trees
errors_hundredtrees_two <- 0
for (set in 1:1000) {
  errors_hundredtrees_two[set] <- forests_two[[set]][[3]][["test"]][["err.rate"]][[100]]
}

c(mean(errors_onetree_two), mean(errors_tentrees_two), mean(errors_hundredtrees_two))
c(var(errors_onetree_two), var(errors_tentrees_two), var(errors_hundredtrees_two))

## 1.3
# Generate 1000 data sets
datasets <- list(list(x=0,
                      y=0))
set.seed(12345)
for (set in 1:1000) {
  x1<-runif(100)
  x2<-runif(100)
  trdata<-cbind(x1,x2)
  y<-as.numeric((x1<0.5 & x2<0.5)|(x1>0.5 & x2>0.5))
  trlabels<-as.factor(y)

  datasets[[set]] <- list(x=trdata,
                      y=trlabels)
}

set.seed(1234)
x1<-runif(1000)
x2<-runif(1000)
tedata<-cbind(x1,x2)
y<-as.numeric((x1<0.5 & x2<0.5)|(x1>0.5 & x2>0.5))
telabels<-as.factor(y)
plot(x1,x2,col=(y+1))

trees <- c(1,10,100)
forests_three <- list(list(list()))
set.seed(12345)
for (set in 1:1000) {
  forests_three[[set]] <- list()
  for (ntrees in 1:3) {
    forests_three[[set]][[ntrees]] <- randomForest(x = datasets[[set]]$x,
                                                 y = datasets[[set]]$y,
                                                 xtest = tedata,
                                                 ytest = telabels,
                                                 ntree = trees[ntrees],
                                                 nodesize = 12,
                                                 keep.forest = TRUE)
  }
}

# Misclassification  with 1 tree
errors_onetree_three <- 0
for (set in 1:1000) {
  errors_onetree_three[set] <- forests_three[[set]][[1]][["test"]][["err.rate"]][[1]]
}

# Misclassification with 10 trees
errors_tentrees_three <- 0
for (set in 1:1000) {
  errors_tentrees_three[set] <- forests_three[[set]][[2]][["test"]][["err.rate"]][[10]]
}

# Misclassification with 100 trees
errors_hundredtrees_three <- 0
for (set in 1:1000) {
  errors_hundredtrees_three[set] <- forests_three[[set]][[3]][["test"]][["err.rate"]][[100]]
}

c(mean(errors_onetree_three), mean(errors_tentrees_three), mean(errors_hundredtrees_three))
c(var(errors_onetree_three), var(errors_tentrees_three), var(errors_hundredtrees_three))


################################
#Assignment 2
################################
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 = 3) # true mixing coefficients
true_mu <- matrix(nrow=3, ncol=D) # true conditional distributions
true_pi=c(1/3, 1/3, 1/3)
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", col="blue", ylim=c(0,1))
points(true_mu[2,], type="o", col="red")
points(true_mu[3,], type="o", col="green")

# Producing the training data
for(n in 1:N) {
  k <- sample(1:3,1,prob=true_pi)
  for(d in 1:D) {
    x[n,d] <- rbinom(1,1,true_mu[k,d])
  }
}

EM <- function(k){
  set.seed(123456789)
  K <- k
  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


  # Random initialization of the parameters
  pi <- runif(K,0.49,0.51)
  pi <- pi / sum(pi)
  for(k in 1:K) {
    mu[k,] <- runif(D,0.49,0.51)
  }

  colors <- c('red','blue','green','yellow')

  for(it in 1:max_it) {

    # E-step: Computation of the fractional component assignments
    for(n in 1:N){
      for(k in 1:K){
        z[n,k] <- pi[k] %*% prod((mu[k,] ^ x[n,]) * ((1-mu[k,]) ^ (1 - x[n,])))
      }
    }
    z <- z / rowSums(z)
    n_k <- colSums(z)
    x_mean_k <- (t(z) %*% x)/n_k


    # Log Likelihood Calculation
    #llik[it] <- sum(t(z) %*% (matrix(log(pi),ncol=K, nrow=N, byrow=TRUE)+
                               #(x %*% t(log(mu)) + (1-x) %*% t(log(1-mu)))))

    llk = 0
    for(i in 1:N){
      for(j in 1:K){
        llk_inner = 0
        for(d in 1:D){
          llk_inner = llk_inner+(x[i,d]*log(mu[j,d])+(1-x[i,d])*log(1-mu[j,d]))
        }
        llk = llk+(z[i,j]) * (log(pi[j])+llk_inner)
      }
    }

    llik[it] = llk
    #cat("iteration: ", it, "log likelihood: ", llik[it], "\n")
    #flush.console()
    # Stop if the log likelihood has not changed significantly
    if(it > 1){
      if((llik[it] - llik[it-1]) <= 0.1){
          break
        }
    }

    #M-step: ML parameter estimation from the data and fractional component assignments

    mu <- x_mean_k
    pi <- n_k/sum(n_k)
  }
  print(pi)
  print(mu)
  plot(mu[1,], type="o", col=colors[1], ylim=c(0,1))
  for(p in 2:K){
    points(mu[p,], type="o",col = colors[p])
  }
  plot(llik[1:it], type="o")
}

trees <- c(1,10,100)
forests_three <- list(list(list()))
set.seed(12345)
for (set in 1:1000) {
  forests_three[[set]] <- list()
  for (ntrees in 1:3) {
    forests_three[[set]][[ntrees]] <- randomForest(x = datasets[[set]]$x,
                                                 y = datasets[[set]]$y,
                                                 xtest = tedata,
                                                 ytest = telabels,
                                                 ntree = trees[ntrees],
                                                 nodesize = 12,
                                                 keep.forest = TRUE)
  }
}

EM(2)
EM(3)
EM(4)

################################
#Assignment 3
################################

## 3.1
library(tidyverse)
library(pamr)
library(ggplot2)
library(mgcv)
library(glmnet)
```

```r
set.seed(12345)
data = read.csv("geneexp.csv")

splitData <- function(data, trainRate) {
  n <- dim(data)[1]
  idxs <- sample(1:n, floor(trainRate*n))
  train <- data[idxs,]
  test <- data[-idxs,]
  return (list(train = train, test = test))
}

split <- splitData(data, 0.7)
train <- split$train
test  <- split$test
y <- train[[ncol(train)]]
x <- t(train[,c(-1,-ncol(train))])
mydata <- list(
  x = x,
  y = as.factor(as.character(y)),
  geneid = as.character(1:nrow(x)),
  genenames = rownames(x)
)

# Training and cross-validating threshold
model <- pamr.train(mydata)
cvmodel <- pamr.cv(model, mydata)

#grDevices::dev.new()
best_threshold = cvmodel$threshold[which.min(cvmodel$error)]
#pamr.plotcen(bestModel, mydata, threshold = best_thresbold)
bestModel <- pamr.train(mydata, threshold = best_threshold)

selectedGenes <- pamr.listgenes(bestModel, mydata,
                                threshold=best_threshold,
                                genenames = TRUE)

cat("the number of selected genes is:",length(unique(selectedGenes[,2])))

#grDevices::dev.new()
pamr.plotcv(cvmodel)
print(cvmodel)
best_threshold = cvmodel$threshold[which.min(cvmodel$error)]
bestModel <- pamr.train(mydata, threshold = best_threshold)
#grDevices::dev.new()

cat("the best threshod is: ", best_threshold)

## 3.2
yTest <- test[[ncol(test)]]
xTest <- t(test[,c(-1,-ncol(test))])
predictions <- pamr.predict(bestModel, newx = xTest, type = "class",
                            threshold = best_threshold)
table(predictions,yTest)
```

```r
tt <-selectedGenes[,2]
cat("2 most repeated genes:",tt[1],tt[2],"\n")
cat("the name ENSG00000204287 Gene is  HLA-DRA and this gene is a marker. ","\n")
cat("The name of ENSG00000019582 Gene is CD74 and this gene is a marker.")

cat("test error for NSC : ",1-sum(diag(table(yTest,predictions)))/length(predictions))

## 3.3
cvElastNet <- cv.glmnet(x=t(x), y=y, alpha=0.5, type.measure = "mse",family="multinomial")
grDevices::dev.new()
plot(cvElastNet)
optLamdba <- cvElastNet$lambda.min
print("optimal lambda:")
optLamdba

elasticnetModel <- glmnet(x = t(x), y = y, family="multinomial",
                          alpha=0.5, lambda = optLamdba)
predictionsElast <- predict(elasticnetModel, newx = t(xTest), type="class")
table(yTest, predictionsElast)
cat("test error: ",1-sum(diag(table(predictionsElast,yTest)))/length(predictionsElast))
coeffs <- coef(elasticnetModel)
nonzeroCoeffsCD19 <- coeffs[which(coeffs$CD19 != 0)]
selectedCoeffsCD19 <- length(nonzeroCoeffsCD19)

nonzeroCoeffsCD4 <- coeffs[which(coeffs$CD4 != 0)]
selectedCoeffsCD4 <- length(nonzeroCoeffsCD4)

nonzeroCoeffsCD8 <- coeffs[which(coeffs$CD8 != 0)]
selectedCoeffsCD8 <- length(nonzeroCoeffsCD8 )

cat("Elasticnet model has ", selectedCoeffsCD4, " nonzero coefficients for CD4\n")
cat("Elasticnet model has ", selectedCoeffsCD19, " nonzero coefficients for CD19\n")
cat("Elasticnet model has ", selectedCoeffsCD8, " nonzero coefficients for CD8\n")

library(kernlab)
library(dplyr)
library(tidyr)
data <-  read.csv("geneexp.csv")

names(train)[ncol(train)] <- "Celltype"
str(train$Celltype)
train$Celltype <- as.factor(train$Celltype)
for (i in 2:2086) {
  train[,i] <- as.numeric(train[,i])
}

svmModel <- ksvm(Celltype ~., data=train[,-1], kernel="vanilladot", scaled=FALSE)
svmPredictions <- predict(svmModel, test)

cat("SVM table \n")
print(table(yTest,svmPredictions))

cat("\n test error for SVM: ",1-sum(diag(table(yTest,svmPredictions)))/length(svmPredictions))
```

```
## 3.4
data = read.csv("geneexp.csv")
y <- as.factor(data[,ncol(data)])
data <- as.matrix(data[,c(-1,-ncol(data))])
data <- data[,-c(43, 69, 179, 188, 217, 384, 527, 540, 600, 647, 1044, 1146, 1330, 1370, 1435, 1505, 19


y1 <- as.factor(as.numeric(y=="CD4"))

pvals1 <- as.numeric(vector(length = ncol(data)))
df <- data.frame(
  word = colnames(data),
  pvals <- pvals1
)
BH1 <- as.numeric(vector(length =ncol(data)))

FDR <- 0.5
CL  <- 0.95



for(i in 1:length(pvals1)) {
  test <- t.test(data[,i]~y1,
                 alternative = "two.sided",
                 conf.level = CL )
  df[i,2] <- test$p.value
  BH1[i] <- (FDR * i / length(pvals1))
}

# order increasingly the pvalues
df <- df[order(df$pvals, decreasing = FALSE),]
df <- cbind(df, BH1)
L <- max(which(df[,2] < df[,3]))
df$reject <- c(rep("Rejected",L), rep("Accepted",(2064-L)))


ggplot() +
  geom_point(aes(x=1:nrow(df), y=df[,2], color=df$reject)) +
  geom_vline(xintercept = L)
cat("number of Rejected Features CD4 =", L, "\n")



y2 <- as.factor(as.numeric(y=="CD8"))

pvals2 <- as.numeric(vector(length = ncol(data)))
df2 <- data.frame(
  word = colnames(data),
  pvals <- pvals2
)
BH2 <- as.numeric(vector(length =ncol(data)))

FDR <- 0.5
```

```r
CL  <- 0.95



for(i in 1:length(pvals2)) {
  test <- t.test(data[,i]~y2,
                 alternative = "two.sided",
                 conf.level = CL )
  df2[i,2] <- test$p.value
  BH2[i] <- (FDR * i / length(pvals2))
}

# order increasingly the pvalues
df2 <- df2[order(df2$pvals, decreasing = FALSE),]
df2 <- cbind(df2, BH2)
L2 <- max(which(df2[,2] < df2[,3]))
df2$reject <- c(rep("Rejected",L2), rep("Accepted",(2064-L2)))


ggplot() +
  geom_point(aes(x=1:nrow(df2), y=df[,2], color=df2$reject)) +
  geom_vline(xintercept = L2)
cat("number of Rejected Features CD8: ", L2, "\n" )

y3 <- as.factor(as.numeric(y=="CD19"))

pvals3 <- as.numeric(vector(length = ncol(data)))
df3 <- data.frame(
  word = colnames(data),
  pvals <- pvals3
)
BH3 <- as.numeric(vector(length =ncol(data)))

FDR <- 0.5
CL  <- 0.95



for(i in 1:length(pvals3)) {
  test <- t.test(data[,i]~y3,
                 alternative = "two.sided",
                 conf.level = CL )
  df3[i,2] <- test$p.value
  BH3[i] <- (FDR * i / length(pvals3))
}

# order increasingly the pvalues
df3 <- df3[order(df3$pvals, decreasing = FALSE),]
df3 <- cbind(df3, BH3)
L3 <- max(which(df3[,2] < df3[,3]))
df3$reject <- c(rep("Rejected",L3), rep("Accepted",(2064-L3)))
```

```
ggplot() +
  geom_point(aes(x=1:nrow(df3), y=df3[,2], color=df3$reject)) +
  geom_vline(xintercept = L3)
cat("Rejected Features CD19: ", L3 ,"\n")
```