Assignment 02

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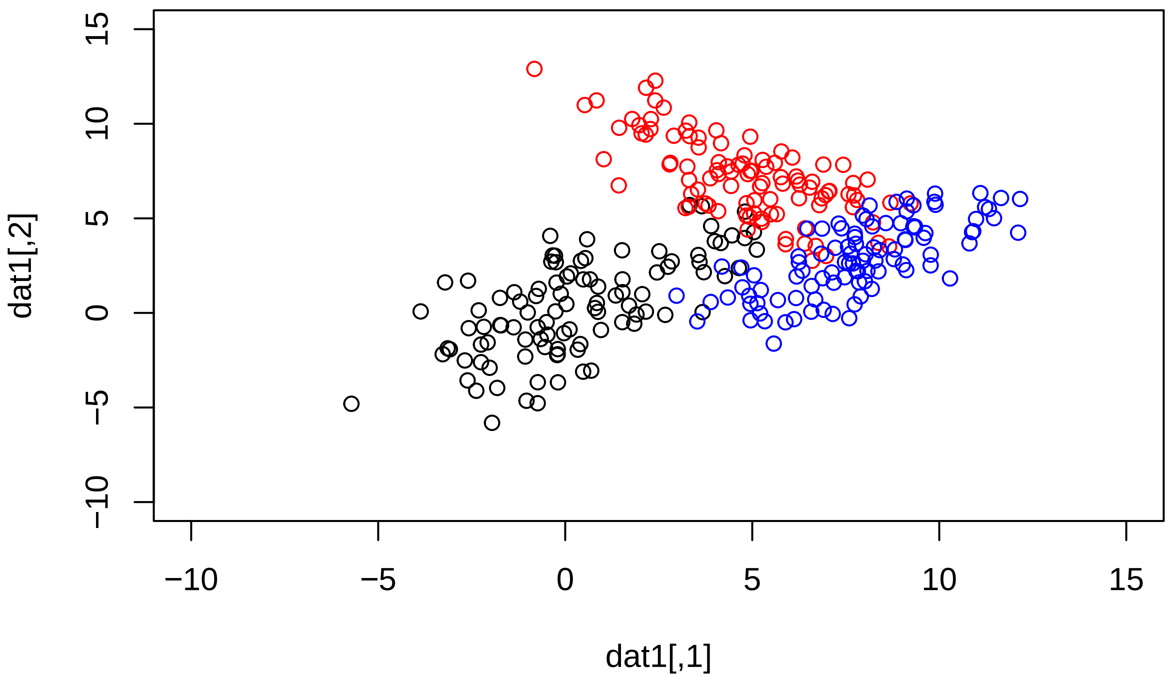
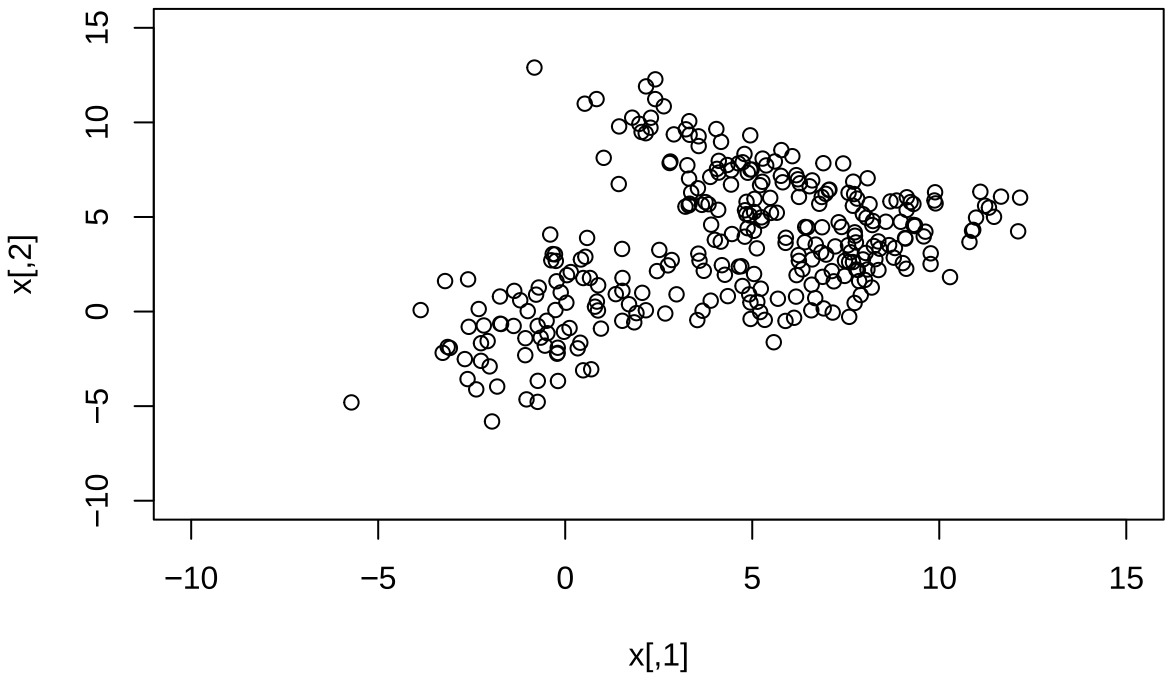
Gaussian Mixture Models

```r
#install.packages("mvtnorm")
library(mvtnorm)
set.seed(1234567890)
min_change <- 0.001 # min parameter change between two consecutive iterations
N=300 # number of training points
D=2 # number of dimensions
x <- matrix(nrow=N, ncol=D) # training data

# Producing the training data
mu1<-c(0,0)
Sigma1 <- matrix(c(5,3,3,5),D,D)
dat1<-rmvnorm(n = 100, mu1, Sigma1)
mu2<-c(5,7)
Sigma2 <- matrix(c(5,-3,-3,5),D,D)
dat2<-rmvnorm(n = 100, mu2, Sigma2)
mu3<-c(8,3)
Sigma3 <- matrix(c(3,2,2,3),D,D)
dat3<-rmvnorm(n = 100, mu3, Sigma3)
plot(dat1,xlim=c(-10,15),ylim=c(-10,15))
points(dat2,col="red")
points(dat3,col="blue")
```



```
x[1:100,]<-dat1
x[101:200,]<-dat2
x[201:300,]<-dat3
plot(x,xlim=c(-10,15),ylim=c(-10,15))
```



```
K=3 # number of classes

w <- matrix(nrow=N, ncol=K) # fractional class assignments
pi <- vector(length=K) # mixing coefficients
mu <- matrix(nrow=K, ncol=D) # class conditional means
Sigma <- array(dim=c(D,D,K)) # class conditional covariances
```

```r
# Calculate pi, mu, and Sigma according to 10.3 page 205
# (assuming the we know the true class of the first ten components of each class)
pi <- c(10, 10, 10) # We know the first 10 components of each class
pi <- pi/sum(pi) # to get percentages
mu[1,] <- colMeans(x[1:10,]) #Mean of the known components for each class
mu[2,] <- colMeans(x[101:110,])
mu[3,] <- colMeans(x[201:210,])
Sigma[,,1] <- var(x[1:10,]) #Variance of the known components for each class
Sigma[,,2] <- var(x[101:110,])
Sigma[,,3] <- var(x[201:210,])
#which is the same as (t(x[1:10,] - mu[1,]) %*% (x[1:10,] - mu[1,])) / 10

pi
```

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

```r
mu
```

```
##             [,1]     [,2]
## [1,] 0.8053535 0.860496
## [2,] 4.1857881 7.206610
## [3,] 7.6752711 2.489227
```

```r
Sigma
```

```
## , , 1
##
##           [,1]     [,2]
## [1,] 7.973370 5.615974
## [2,] 5.615974 6.797121
##
## , , 2
##
##            [,1]      [,2]
## [1,]  2.015831 -1.486711
## [2,] -1.486711  3.692204
##
## , , 3
##
##           [,1]     [,2]
## [1,] 4.708158 2.535410
## [2,] 2.535410 2.811314
```

```r
# set max_it to some value
max_it <- 10000
llik <- rep(NA, length=max_it) #Create vector to store log-likelihoods which is
# needed to compare the minimum change in log-likelihoods.
for (it in 1:max_it) {
  # E-step: Computation of the fractional component
  # assignments
  llik[it] <- 0
  for (n in 1:N) { # According to the instructions, the algorithm is not run
    # for all value of N data points but only for the unkown ones. This does not
    # make a difference though, because in the implementation below every known
    # data point is set to its original known value (i.e. 1 for the correct
    # class and 0 for the incorrect ones). In other words, these iterations do
    # not make a difference and it is the same as if they were set only one
    # initial time.
    for (k in 1:K) {
      w[n, k] <- pi[k] * dmvnorm(x[n, ], mu[k, ], Sigma[,, k])
    }
    # If data point is known, set to 1 for correct class and 0 for all others
    if (n %in% 1:10){
      w[n,1] <- 1
      w[n,2] <- 0
      w[n,3] <- 0
    }
    if (n %in% 101:110){
      w[n,1] <- 0
      w[n,2] <- 1
      w[n,3] <- 0
    }
    if (n %in% 201:210){
      w[n,1] <- 0
      w[n,2] <- 0
      w[n,3] <- 1
    }
    # Log likelihood computation.
    llik[it] <- llik[it] + log(sum(w[n, ]))
    w[n, ] <- w[n, ]/sum(w[n, ]) # does not change value of known data points
    # because they sum up to one by definition
  }
  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
  for (k in 1:K) { # for each class calculate
    pi[k] <- sum(w[, k])/N # pi according to (10.10b)
    for (d in 1:D) { # for each dimension calculate
      mu[k, d] <- sum(x[, d] * w[, k])/sum(w[, k]) # mu according to (10.10c)
    }
    for (d in 1:D) { # for each dimension calculate
      for (d2 in 1:D) { # for each dimension calculate
        Sigma[d, d2, k] <- sum((x[, d] - mu[k, d]) * (x[, d2] - mu[k, d2]) *
                             w[, k])/sum(w[, k])
        # according to (10.10d)
      }
    }
  }
}
```

```
## iteration:  1 log likelihood:  -1376.92
## iteration:  2 log likelihood:  -1346.474
## iteration:  3 log likelihood:  -1342.466
## iteration:  4 log likelihood:  -1341.037
## iteration:  5 log likelihood:  -1340.37
## iteration:  6 log likelihood:  -1339.997
## iteration:  7 log likelihood:  -1339.761
## iteration:  8 log likelihood:  -1339.602
## iteration:  9 log likelihood:  -1339.488
## iteration:  10 log likelihood:  -1339.405
## iteration:  11 log likelihood:  -1339.343
## iteration:  12 log likelihood:  -1339.296
## iteration:  13 log likelihood:  -1339.26
## iteration:  14 log likelihood:  -1339.232
## iteration:  15 log likelihood:  -1339.21
## iteration:  16 log likelihood:  -1339.194
## iteration:  17 log likelihood:  -1339.18
## iteration:  18 log likelihood:  -1339.17
## iteration:  19 log likelihood:  -1339.162
## iteration:  20 log likelihood:  -1339.155
## iteration:  21 log likelihood:  -1339.15
## iteration:  22 log likelihood:  -1339.146
## iteration:  23 log likelihood:  -1339.143
## iteration:  24 log likelihood:  -1339.14
## iteration:  25 log likelihood:  -1339.138
## iteration:  26 log likelihood:  -1339.136
## iteration:  27 log likelihood:  -1339.135
## iteration:  28 log likelihood:  -1339.134
## iteration:  29 log likelihood:  -1339.133

## [1] "Actual mu values"

##      [,1] [,2]
## [1,]    0    0
## [2,]    5    7
## [3,]    8    3

## [1] "GMM mu values (rounded to 2 decimal places"

##      [,1] [,2]
## [1,] 0.26 0.25
## [2,] 4.94 7.02
## [3,] 7.76 2.89

## [1] "Actual Sigma values"

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

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

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

## [1] "GMM Sigma values"

## , , 1
```

```
##
##          [,1]     [,2]
## [1,] 5.154362 3.637591
## [2,] 3.637591 6.450587
##
## , , 2
##
##           [,1]      [,2]
## [1,]  4.440287 -3.256524
## [2,] -3.256524  4.889810
##
## , , 3
##
##          [,1]     [,2]
## [1,] 4.052096 2.756186
## [2,] 2.756186 3.803429
```

```
## [1] "Actual pi values"
```

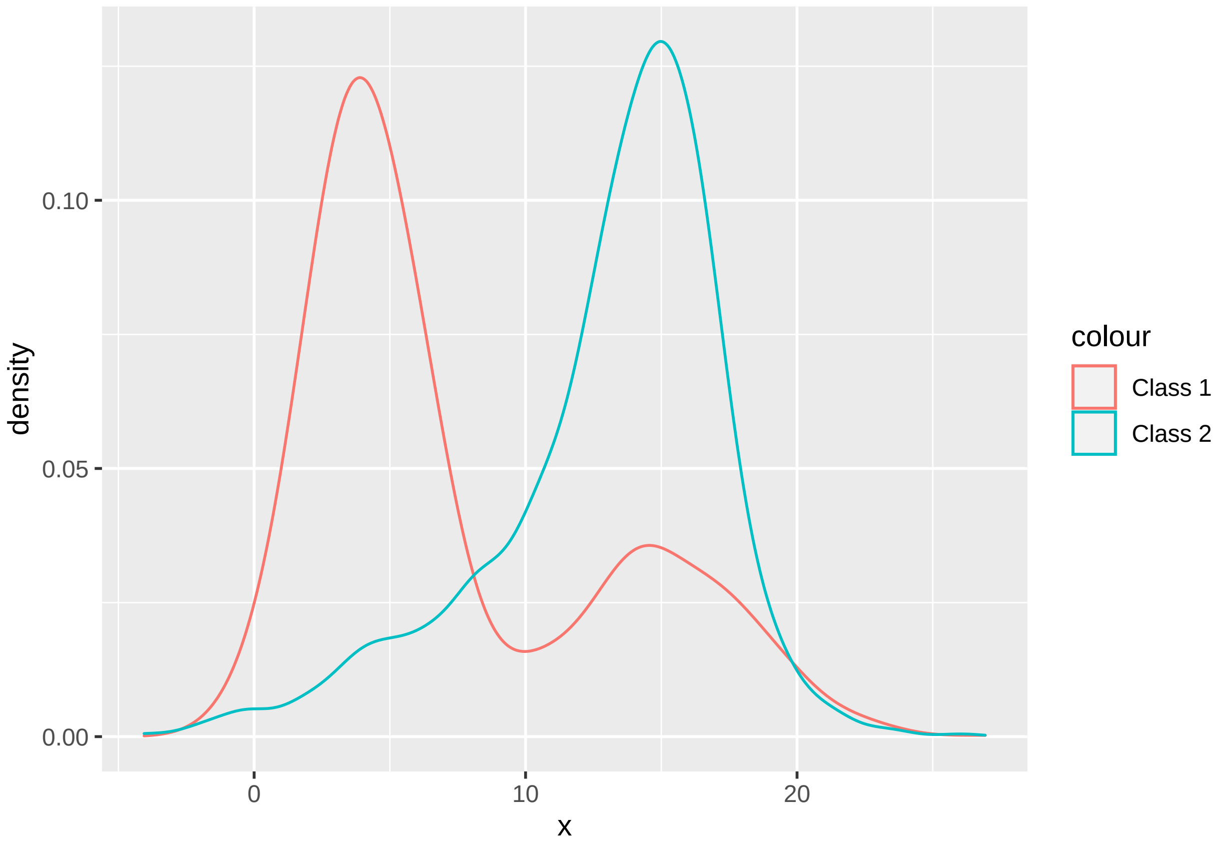
```
## [1] 0.3333333 0.3333333 0.3333333
```

```
## [1] "GMM Sigma values"
```

```
## [1] 0.3273498 0.3470995 0.3255508
```

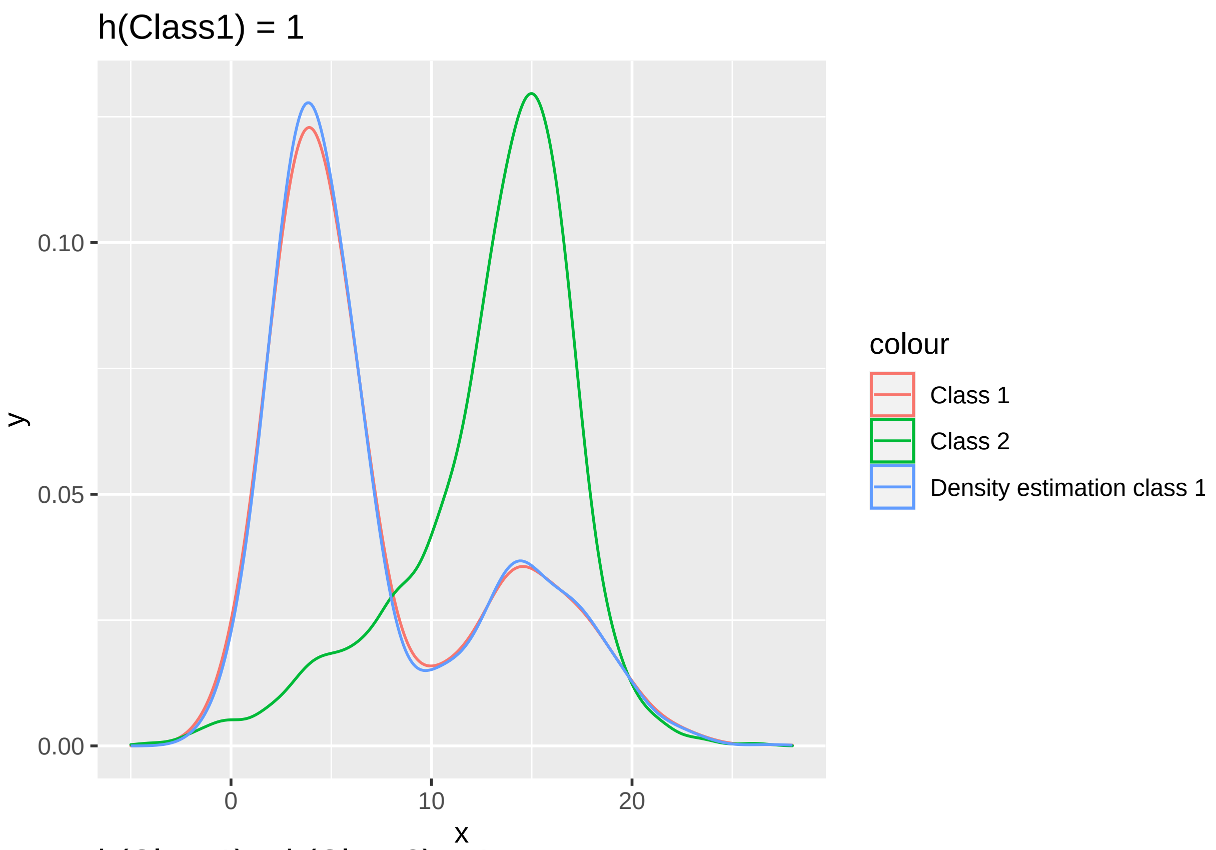
The values of mu, Sigma, and pi are close to the original ones. If the estimated mu values were rounded to a whole number, all of the estimations would perfectly fit the actual mu values. This is also true for most of the Sigma values. The pi values also almost perfectly show the even distribution of the three classes in the sense the actual three class labels belonged to one third of the data points each.
One can also see that the log-likelihood strictly increases up until the convergence criterion is reached.

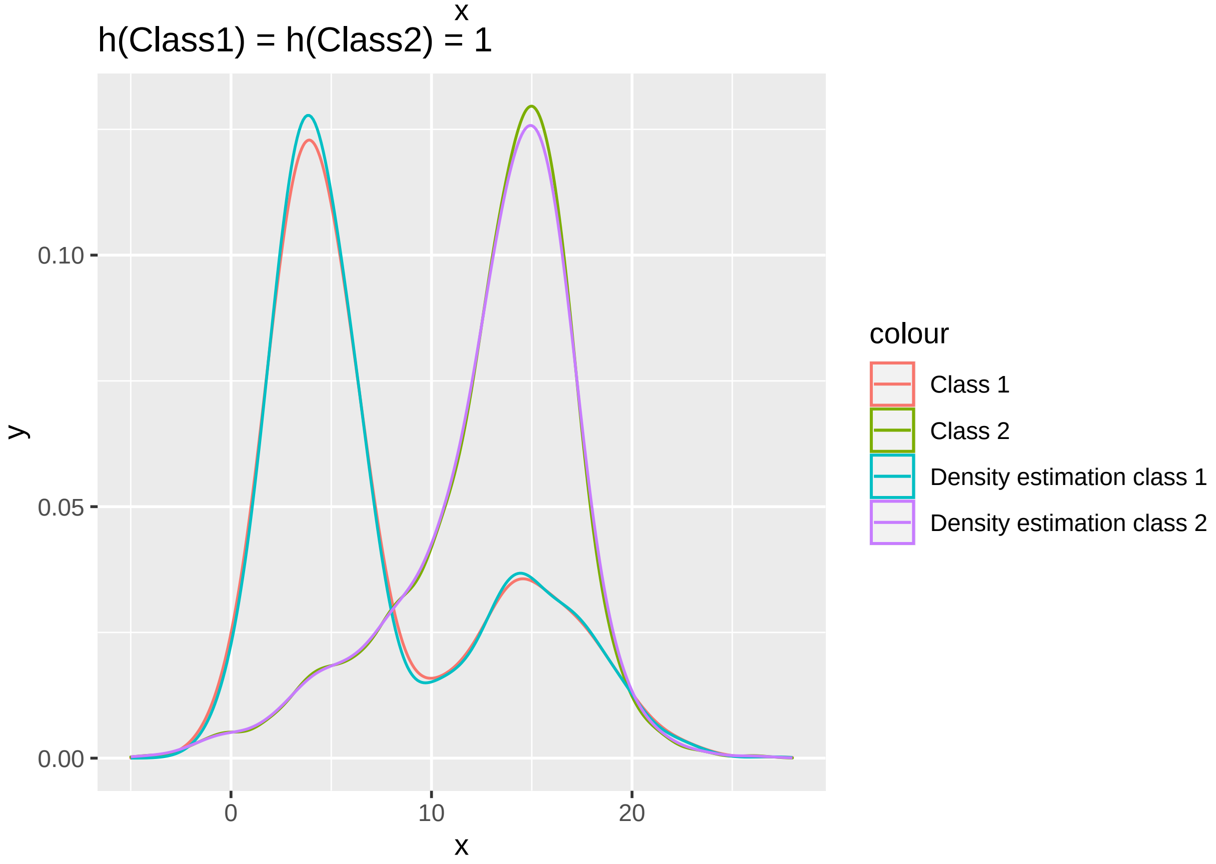
Kernel Models



```
create_estimated_density <- function(data, h){ # returns the estimated density
  # function according to the instructions for the given data and a value of h
  res <- function(x){
    dists <- x - data
    dists <- dists / h # The larger h, the smaller get the dists values
    return(mean(dnorm(dists))) # the smaller the dists value, the higher the
    # value of dnorm(dists)
  }
  return(res)
}
```

In the plot above one can see the density estimation of the data of the build in `geom_density` function of the ggplot2 package. It is nice as a comparison, as it is implemented in a way that the integral sums up to one which should be true for densities by definition.
This condition is not automatically true for all values of h. If one considers, for example, that h would be infinity, all the kernels would have the value dnorm(0) $= 0.3989423$ for all input values x^* and therefore the integral over all these values would be infinity, not one.
A value of h has to be chosen to make the integral over the estimated densities as close to 1 as possible. The ggplot function `geom_density` can therefore be helpful.





One can see that if both values of h are chosen to be 1, the fit to the ggplot density seems to be quite good and the integral over all values of x therefore close to 1. This means that h = 1 is a good value for both data_class1 and data_class2.

To get the probability of a class (e.g. class 1) given a value of x_* on could use Bayes Theorem which states that $P(Class = 1|x_*) = \frac{P(x_*|Class=1)P(Class=1)}{P(x_*)}$ where $P(x_*|Class = 1)$ is the function derived above, $P(Class = 1)$ is the probability of any point being in class one (so it is the proportion of data points falling in class 1, here 1500/(1000+1500) = 0.6 which is from now on called weight of class 1 or in general w_i for class i) and $P(x_*)$ is the weighted sum of the functions $P(x_*|Class = i)$ so $P(x_*) = w_1P(x_*|Class = 1) + w_2P(x_*|Class = 2)$.

In total this results in $P(Class = 1|x_*) = \frac{P(x_*|Class=1)\cdot 0.6}{0.6P(x_*|Class=1)+0.4P(x_*|Class=2)}$
for class 1 and $P(Class = 2|x_*) = \frac{P(x_*|Class=2)\cdot 0.4}{0.6P(x_*|Class=1)+0.4P(x_*|Class=2)}$
for class 2.

Appendix

```r
#install.packages("mvtnorm")
library(mvtnorm)
set.seed(1234567890)
min_change <- 0.001 # min parameter change between two consecutive iterations
N=300 # number of training points
D=2 # number of dimensions
x <- matrix(nrow=N, ncol=D) # training data

# Producing the training data
mu1<-c(0,0)
Sigma1 <- matrix(c(5,3,3,5),D,D)
dat1<-rmvnorm(n = 100, mu1, Sigma1)
mu2<-c(5,7)
Sigma2 <- matrix(c(5,-3,-3,5),D,D)
dat2<-rmvnorm(n = 100, mu2, Sigma2)
mu3<-c(8,3)
Sigma3 <- matrix(c(3,2,2,3),D,D)
dat3<-rmvnorm(n = 100, mu3, Sigma3)
plot(dat1,xlim=c(-10,15),ylim=c(-10,15))
points(dat2,col="red")
points(dat3,col="blue")
x[1:100,]<-dat1
x[101:200,]<-dat2
x[201:300,]<-dat3
plot(x,xlim=c(-10,15),ylim=c(-10,15))
K=3 # number of classes

w <- matrix(nrow=N, ncol=K) # fractional class assignments
pi <- vector(length=K) # mixing coefficients
mu <- matrix(nrow=K, ncol=D) # class conditional means
Sigma <- array(dim=c(D,D,K)) # class conditional covariances

# Calculate pi, mu, and Sigma according to 10.3 page 205
# (assuming the we know the true class of the first ten components of each class)
pi <- c(10, 10, 10) # We know the first 10 components of each class
pi <- pi/sum(pi) # to get percentages
mu[1,] <- colMeans(x[1:10,]) #Mean of the known components for each class
mu[2,] <- colMeans(x[101:110,])
mu[3,] <- colMeans(x[201:210,])
```

```r
Sigma[,,1] <- var(x[1:10,]) #Variance of the known components for each class
Sigma[,,2] <- var(x[101:110,])
Sigma[,,3] <- var(x[201:210,])
#which is the same as (t(x[1:10,] - mu[1,]) %*% (x[1:10,] - mu[1,])) / 10

pi
mu
Sigma
# set max_it to some value
max_it <- 10000
llik <- rep(NA, length=max_it) #Create vector to store log-likelihoods which is
# needed to compare the minimum change in log-likelihoods.
for (it in 1:max_it) {
  # E-step: Computation of the fractional component
  # assignments
  llik[it] <- 0
  for (n in 1:N) { # According to the instructions, the algorithm is not run
    # for all value of N data points but only for the unkown ones. This does not
    # make a difference though, because in the implementation below every known
    # data point is set to its original known value (i.e. 1 for the correct
    # class and 0 for the incorrect ones). In other words, these iterations do
    # not make a difference and it is the same as if they were set only one
    # initial time.
    for (k in 1:K) {
      w[n, k] <- pi[k] * dmvnorm(x[n, ], mu[k, ], Sigma[,, k])
    }
    # If data point is known, set to 1 for correct class and 0 for all others
    if (n %in% 1:10){
      w[n,1] <- 1
      w[n,2] <- 0
      w[n,3] <- 0
    }
    if (n %in% 101:110){
      w[n,1] <- 0
      w[n,2] <- 1
      w[n,3] <- 0
    }
    if (n %in% 201:210){
      w[n,1] <- 0
      w[n,2] <- 0
      w[n,3] <- 1
    }
    # Log likelihood computation.
    llik[it] <- llik[it] + log(sum(w[n, ]))
    w[n, ] <- w[n, ]/sum(w[n, ]) # does not change value of known data points
    # because they sum up to one by definition
  }
  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
  for (k in 1:K) { # for each class calculate
    pi[k] <- sum(w[, k])/N # pi according to (10.10b)
    for (d in 1:D) { # for each dimension calculate
      mu[k, d] <- sum(x[, d] * w[, k])/sum(w[, k]) # mu according to (10.10c)
    }
    for (d in 1:D) { # for each dimension calculate
      for (d2 in 1:D) { # for each dimension calculate
        Sigma[d, d2, k] <- sum((x[, d] - mu[k, d]) * (x[, d2] - mu[k, d2]) *
                                 w[, k])/sum(w[, k])
        # according to (10.10d)
      }
    }
  }
}

print("Actual mu values")
matrix(c(mu1, mu2, mu3), nrow=3, ncol=2, byrow = TRUE)
print("GMM mu values (rounded to 2 decimal places")
round(mu, 2)
print("Actual Sigma values")
Sigma1
Sigma2
Sigma3
print("GMM Sigma values")
Sigma
print("Actual pi values")
c(1/3, 1/3, 1/3)
print("GMM Sigma values")
pi

set.seed(1234567890)
N_class1 <- 1500
N_class2 <- 1000
data_class1 <- NULL
for(i in 1:N_class1){
  a <- rbinom(n = 1, size = 1, prob = 0.3)
  b <- rnorm(n = 1, mean = 15, sd = 3) * a + (1-a) * rnorm(n = 1, mean = 4, sd
  = 2)
  data_class1 <- c(data_class1,b)
}
data_class2 <- NULL
for(i in 1:N_class2){
  a <- rbinom(n = 1, size = 1, prob = 0.4)
  b <- rnorm(n = 1, mean = 10, sd = 5) * a + (1-a) * rnorm(n = 1, mean = 15,
  sd = 2)
  data_class2 <- c(data_class2,b)
}
```

```r
library(ggplot2)
ggplot() +
  geom_density(data.frame(x=data_class1), mapping=aes(x, color="Class 1")) +
  geom_density(data.frame(x=data_class2), mapping=aes(x, color="Class 2"))

create_estimated_density <- function(data, h){ # returns the estimated density
  # function according to the instructions for the given data and a value of h
  res <- function(x){
    dists <- x - data
    dists <- dists / h # The larger h, the smaller get the dists values
    return(mean(dnorm(dists))) # the smaller the dists value, the higher the
    # value of dnorm(dists)
  }
  return(res)
}


density_est1 <- create_estimated_density(data_class1, 1)
plot_data1 <- data.frame(x=seq(-5, 28, 0.1), y=sapply(seq(-5, 28, 0.1),
                                                       density_est1))

ggplot() +
  geom_density(data.frame(x=data_class1), mapping=aes(x, color="Class 1")) +
  geom_density(data.frame(x=data_class2), mapping=aes(x, color="Class 2")) +
  geom_line(plot_data1, mapping=aes(x,y, color="Density estimation class 1")) +
  labs(title="h(Class1) = 1")

density_est2 <- create_estimated_density(data_class2, 1)
plot_data2 <- data.frame(x=seq(-5, 28, 0.1), y=sapply(seq(-5, 28, 0.1),
                                                       density_est2))

ggplot() +
  geom_density(data.frame(x=data_class1), mapping=aes(x, color="Class 1")) +
  geom_density(data.frame(x=data_class2), mapping=aes(x, color="Class 2")) +
  geom_line(plot_data1, mapping=aes(x,y, color="Density estimation class 1")) +
  geom_line(plot_data2, mapping=aes(x,y, color="Density estimation class 2")) +
  labs(title="h(Class1) = h(Class2) = 1")
```