Density Estimation

Bandwidht choice by leave-one-out maximum likelihood

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Histogram

1. At the slides we have seen the following relationship

$$\hat{f}_{h,(-i)}(x_i) = \frac{n}{n-1}\left(\hat{f}_h(x_i) - \frac{K(0)}{nh}\right)$$

between the leave-one-out kernel density estimator $\hat{f}_{h,(-i)}(x)$ and the kernel density estimator using all the observations $\hat{f}_h(x)$, when both are evaluated at x_i, one of the observed data. Find a similar relationship between the histogram estimator of the density function $\hat{f}_{hist}(x)$ and its leave-one-out version, $\hat{f}_{hist,(-i)}(x)$, when both are evaluated at x_i.

Starting from the formula for the histogram seen in the slides:

$$\hat{f}_{hist}(x) = \sum_{j=1}^{m} \frac{n_j}{n}\frac{1}{b} I_{B_j}(x)$$

And knowing the following equalities for the single point x_i

$$\hat{f}_{hist}(x_i) = \frac{n_j}{n}\frac{1}{b} \qquad \hat{f}_{hist,(-i)}(x_i) = \frac{n_j - 1}{n-1}\frac{1}{b}$$

We can transform the equation on the left to $n_j = nb\hat{f}_{hist}(x_i)$. Then, we can replace this value of n_j into the equation on the left (loo-cv). This give us then following equations:

$$\hat{f}_{hist,(-i)}(x_i) = \frac{nb\hat{f}_{hist}(x_i) - 1}{n-1}\frac{1}{b}$$

$$\hat{f}_{hist,(-i)}(x_i) = \frac{n\hat{f}_{hist}(x_i)b}{(n-1)b} - \frac{1}{(n-1)b}$$

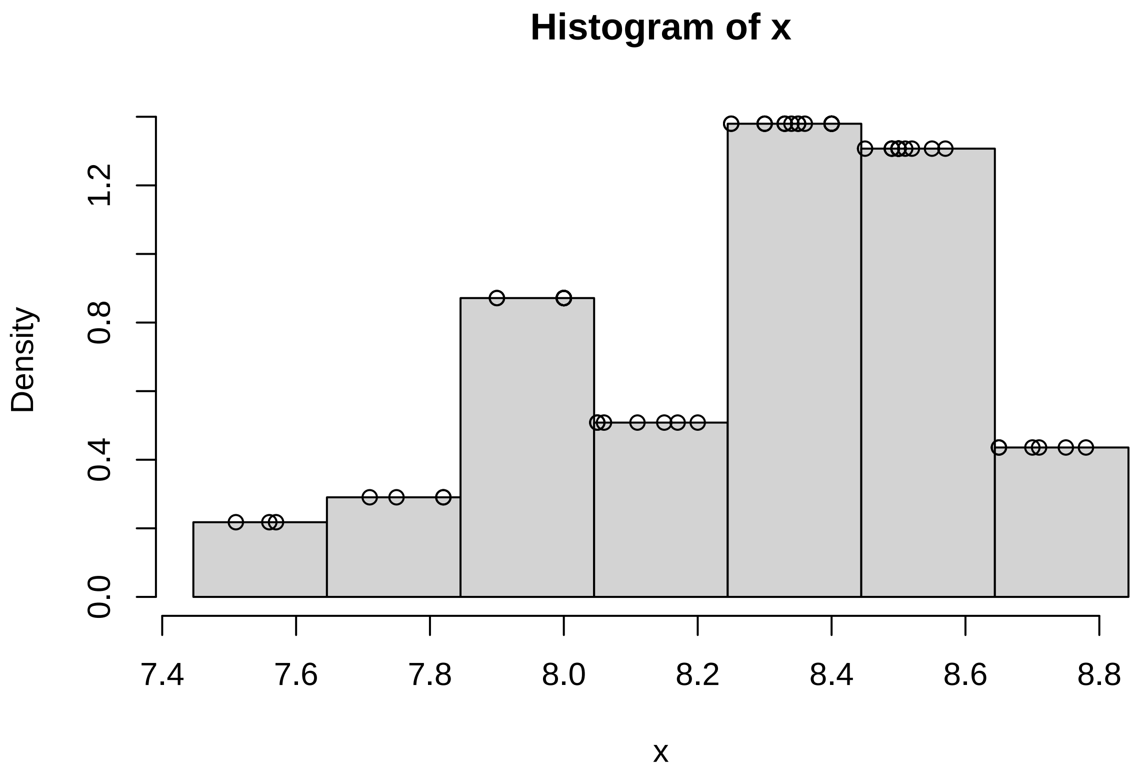
$$\hat{f}_{hist,(-i)}(x_i) = \frac{n}{n-1}\hat{f}_{hist}(x_i) - \frac{1}{(n-1)b}$$

$$\hat{f}_{hist,(-i)}(x_i) = \frac{1}{n-1}\left(n\hat{f}_{hist}(x_i) - \frac{1}{b}\right)$$

2. Read the CD rate data set and call x the first column. Then define A, Z and nbr and plot the histogram of x

```r
cdrate.df <-read.table("./cdrate.dat.txt")
# head(cdrate.df)
x <- cdrate.df[,1]
# sort(CDrate)
# # Stem-and-Leaf plot
# stem(CDrate)
```

```r
A <- min(x)-.05*diff(range(x))
Z <- max(x)+.05*diff(range(x))
nbr <- 7

hx <- hist(x,breaks=seq(A,Z,length=nbr+1),freq=F)
hx_f <- stepfun(hx$breaks,c(0,hx$density,0))
points(x, hx_f(x))
```



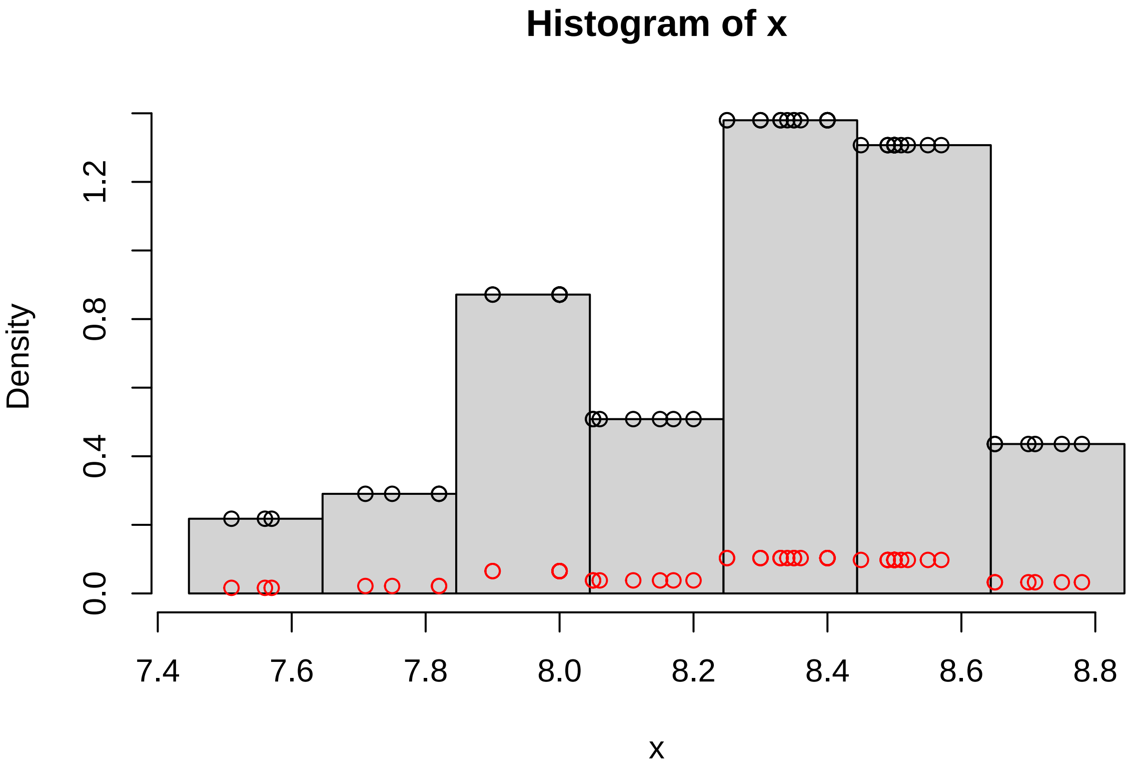
3. Use the formula you have found before relating $\hat{f}_{hist}(x_i)$ and $\hat{f}_{hist,(-i)}(x_i)$ to compute $\hat{f}_{hist,(-i)}(x), i = 1, ..., n,$. Then, add the points $(x_i, \hat{f}_{hist,(-i)}(x_i)), i = 1, ..., n$, to the previous plot.

   In the question 2 we have obtained the next formula:

$$\hat{f}_{hist,(-i)}(x_i) = \frac{n}{n-1}\hat{f}_{hist}(x_i) - \frac{1}{(n-1)b}$$

   We can use it to generate new points that we can compare with the previous plot.

```r
n <- length(x)
b <- hx$breaks[2]-hx$breaks[1]
hx_f2 <- (n/(n-1)* hx_f(x)) * 1/((n-1)*b) # (n/(n-1)* hx_f(x))- 1/((n-1)*b)

A <- min(x)-.05*diff(range(x))
Z <- max(x)+.05*diff(range(x))
nbr <- 7
hx <- hist(x,breaks=seq(A,Z,length=nbr+1),freq=F)
hx_f <- stepfun(hx$breaks,c(0,hx$density,0))
points(x, hx_f(x))
points(x, hx_f2, col="red")
```



4. Compute the leave-one-out log-likelihood function corresponding to the previous histogram, at which *nbr=7* has been used

```r
looCV_log_lik_7 <- sum(log(hx_f2))
looCV_log_lik_7
```

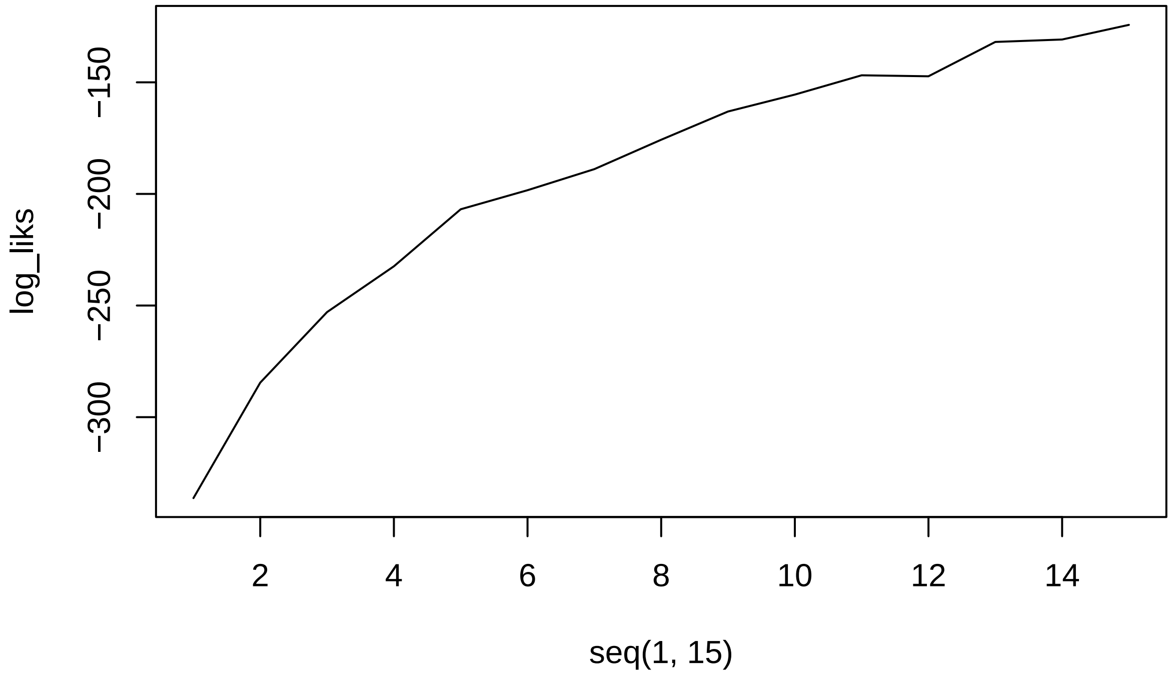
```
## [1] -188.8907
```

5. **Choosing *nbr* by leave-one-out Cross Validation (looCV)**. Consider now the set *seq(1,15)* as possible values for *nbr*, the number of intervals of the histogram. For each of them compute the leave-one-out log-likelihood function (*looCv_log_lik*) for the corresponding histogram. Then plot the values of *looCv_log_lik* against the values of *nbr* and select the optimal value of *nbr* as that at which *looCv_log_lik* takes its maximum. Finally, plot the histogram of x using the optimal value of *nbr*

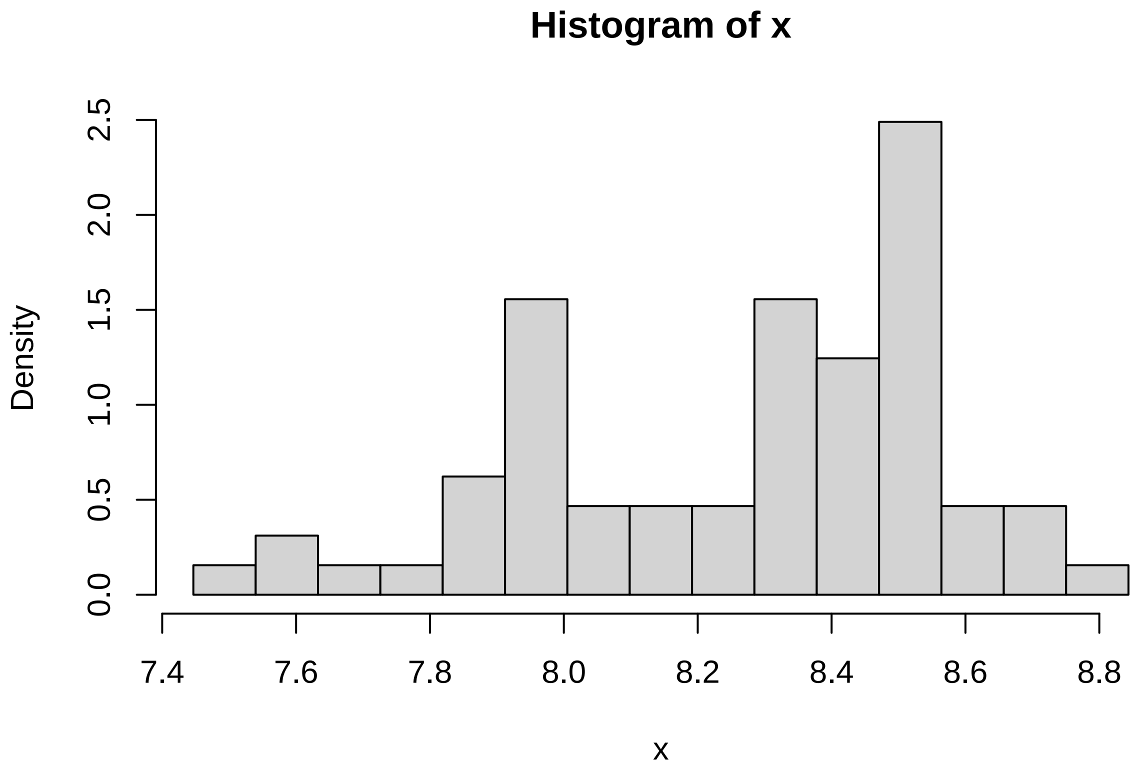
```r
#sum of the product of the hx_f2 vector plot histograms for different number of breaks nbr

log_liks = list()

A <- min(x)-.05*diff(range(x))
Z <- max(x)+.05*diff(range(x))
n <- length(x)

for (nbr in c(1:15)){
  hx_i <- hist(x,breaks=seq(A,Z,length=nbr+1), plot = FALSE)
  hx_f_i <- stepfun(hx_i$breaks,c(0,hx_i$density,0))
  b <- hx_i$breaks[2]-hx_i$breaks[1]
  hx_f2_i <- (n/(n-1)* hx_f_i(x)) * 1/((n-1)*b) # 1/(n-1)*(n*hx_f_i(x) - (1/b))  #(n/(n-1)*hx_f_i(x)) -
  print(min(hx_f2_i))

  #hx_i <- hist(x,breaks=seq(A,Z,length=nbr+1),freq=F)
  #points(x, hx_f_i(x))
  #points(x, hx_f2_i, col='red')

  looCV_log_lik <- sum(log(hx_f2_i)) # TODO: Negative numbers produce NaNs
  log_liks <- append(log_liks, looCV_log_lik)
}
```

```
## [1] 0.007646073
## [1] 0.01019476
## [1] 0.008975825
## [1] 0.008865012
## [1] 0.01108127
## [1] 0.01196777
## [1] 0.01628946
## [1] 0.01418402
## [1] 0.01795165
## [1] 0.01108127
## [1] 0.02681666
## [1] 0.01595702
## [1] 0.01872734
## [1] 0.02171928
## [1] 0.02493285
```

```r
plot(seq(1, 15), log_liks, type = "l")
```



```
nbr_opt <- which.max(log_liks)
hist(x,breaks=seq(A,Z,length=nbr_opt+1),freq=F)
```

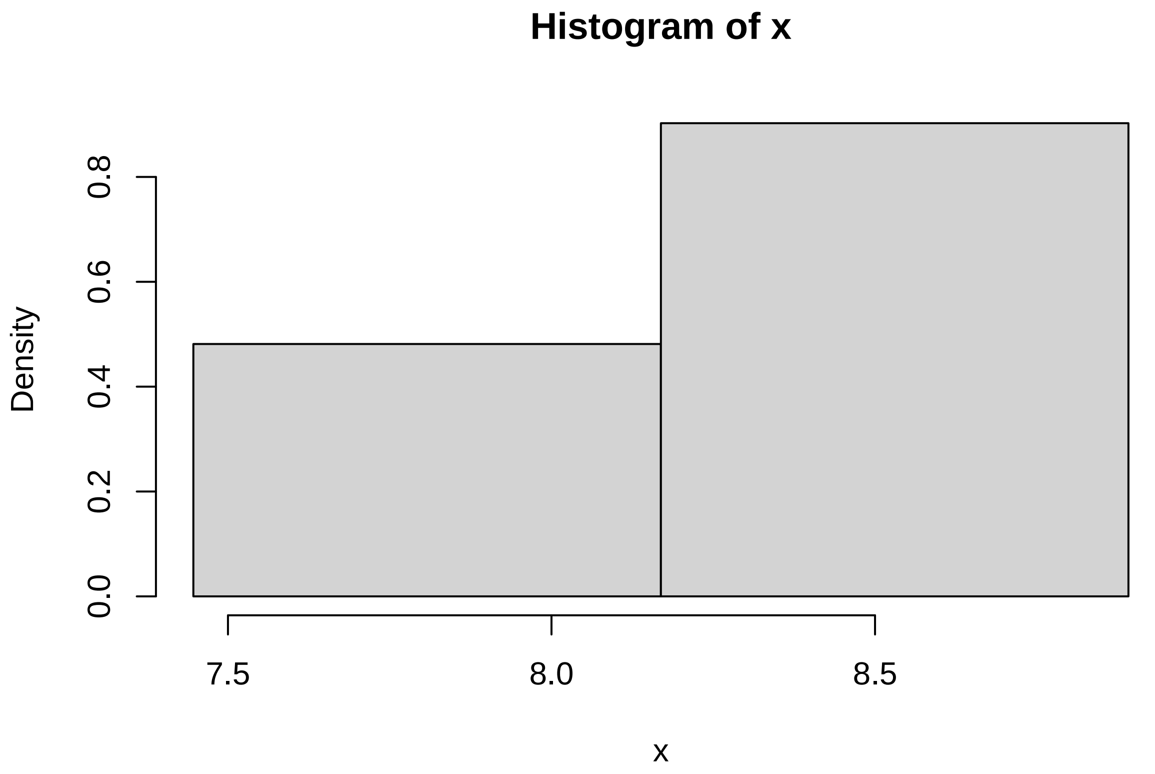


```
# TODO: - avoid production of NaNs,
#       - is it a problem that 'freq' is not used for some cases?
```

6. **Chossing b by looCV**. Let b be the common width of the bins of a histogram. Consider the set $seq((Z-A)/15, (Z-A)/1, length = 30)$ as possible values for b. Select the value of b maximizing the leave-one-out log-likelihood function, and plot the corresponding histogram

```
b_set <- seq((Z-A)/15, (Z-A), length=30)

b_max_log_lik <- function(b_set, x){

  log_liks_b = list()
  n <- length(x)

  for(b in b_set){
    hx <- hist(x, breaks=seq(A, Z+b, by=b), plot=F)

    # compute histogram estimator
    hx_f <- stepfun(hx$breaks,c(0,hx$density,0))
    hx_f2 <- (n/(n-1)* hx_f_i(x)) * 1/((n-1)*b) # 1/(n-1)*(n*hx_f_i(x) - (1/b)) #(n/(n-1)*hx_f_i(x)) - 

    looCV_log_lik_b <- sum(log(hx_f2))
    log_liks_b <- append(log_liks, looCV_log_lik_b)

  }
```

```r
  b_opt <- which.max(log_liks_b)
  b <- b_set[b_opt]
  return(b)
y}

b <- b_max_log_lik(b_set, x)

hx <- hist(x, breaks=seq(A, Z+b, by=b), plot=F)
plot(hx, freq = FALSE)
```



```r
# TODO: avoid NaNs
```

7. Recycle the functions *graph.mixt* and *sim.mixt* defined at *density_estimation.Rmd* to generate n = 100 data from

$$f(x) = (3/4)N(x; m = 0, s = 1) + (1/4)N(x; m = 3/2, s = 1/3)$$

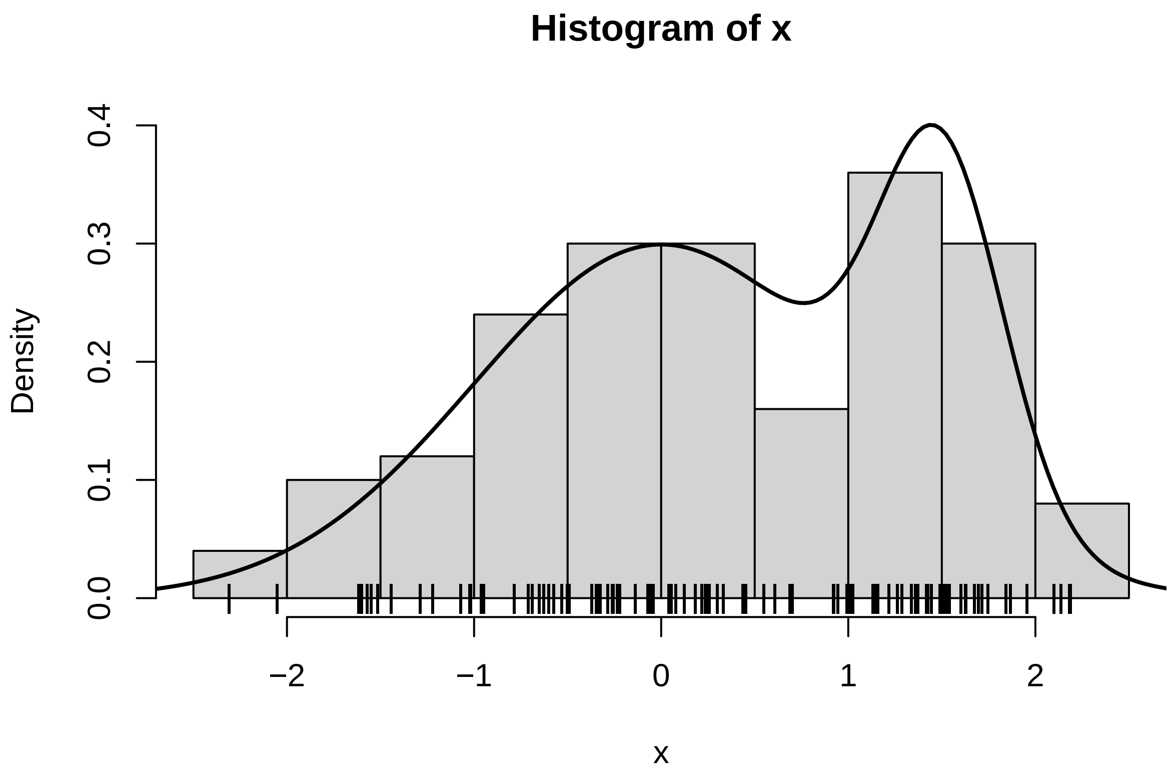
Let b be the bin width of a histogram estimator of f(x) using the generated data. Select the value of b maximizing the leave-one-out log-likelihood function, and plot the corresponding histogram. Compare with the results obtained using the Scott's formula:

$$b_{Scott} = 3.49 St.Dev(X)_n^{-1/3}$$

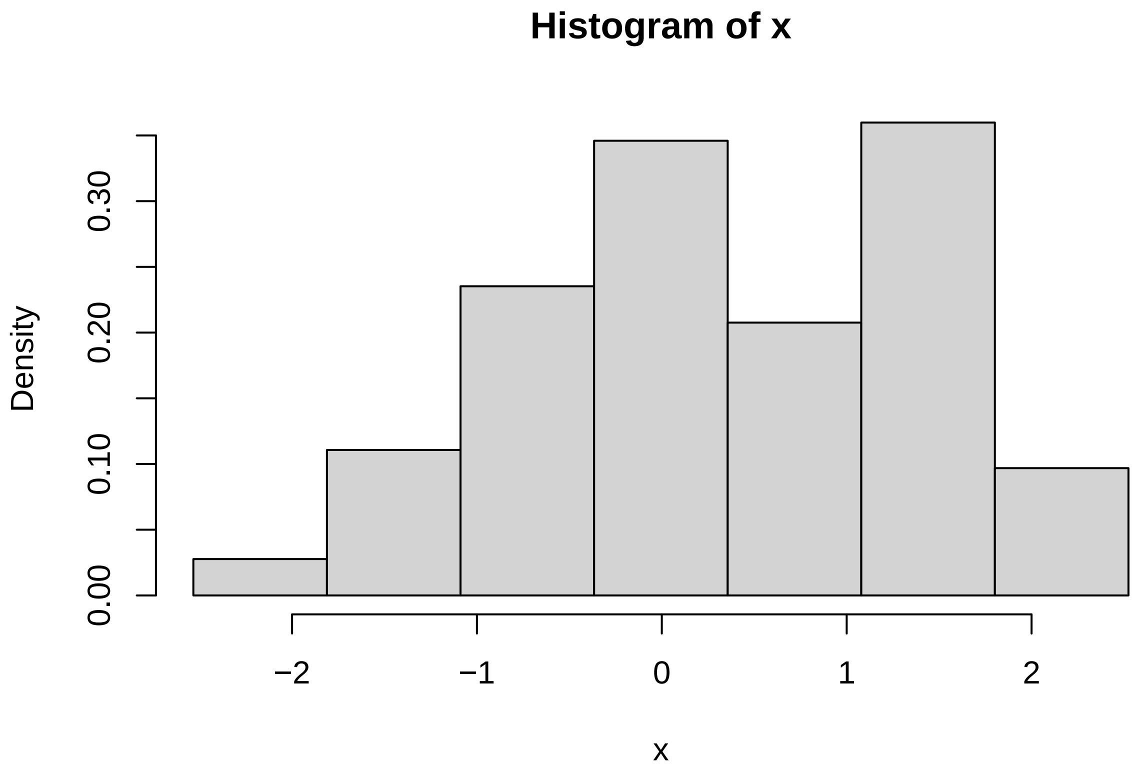
.

```
# graph.mixt
# Input:
#    k: number mixture components
#    mu: vector of length k with the mean values of the k normals
#    sigma: vector of length k with the st.dev. values of the k normals
#    alpha: vector of length k with the weights of each normal
#    graphic: logical value indicating if the mixture density must be plotted
#    ...: Other parameters passed to plot()
#
# Output:
#    L, U: extremes of the interval where the mixture density is plotted
#    x: points at which the mixture density is evaluated
#    fx: value of the mixture density at x
#
graph.mixt<-
function(k=1, mu=seq(-2*(k-1),2*(k-1),length=k), sigma=seq(1,1,length=k), alpha=seq(1/k,1/k,length=k), g
{
   L<-min(mu-3*sigma)
   U<-max(mu+3*sigma)

   x<- seq(from=L,to=U,length=200)
   fx<- 0*x
   Salpha<-sum(alpha)
   for(i in 1:k){
    p<-alpha[i]/Salpha
#       fx <- fx + p*exp(-.5*((x-mu[i])/sigma[i])^2)/(sqrt(2*pi)*sigma[i])
    fx <- fx + p*dnorm(x,mu[i],sigma[i])
   }
   if (graphic){
      plot(x,fx,type="l",...)
   }
   return(list(L = L, U = U, x = x, fx = fx))
}

# sim.mixt
# Input:
#    n: number of simulated data
#    k: number mixture components
#    mu: vector of length k with the mean values of the k normals
#    sigma: vector of length k with the st.dev. values of the k normals
#    alpha: vector of length k with the weights of each normal
#    graphic: logical value indicating if the mixture density and the
#              histogram of the simulated data must be plotted
#    ...: Other parameters passed to plot()
#
# Output:
#    x: simulated data
#
# Requires:
#    graph.mixt
sim.mixt <- function(n=1,k=1,
         mu=seq(-2*(k-1),2*(k-1),length=k),
         sigma=seq(1,1,length=k),
         alpha=seq(1/k,1/k,length=k), graphic=FALSE,...)
{
   csa<-cumsum(alpha)
   x<-runif(n)

   for (i in 1:n){
      comp<-sum(csa<=x[i])+1
      x[i]<-rnorm(1,mu[comp],sigma[comp])
   }
   if(graphic) {
      out<-graph.mixt(k, mu, sigma, alpha, gr=FALSE)
      hist(x,freq = FALSE,
           ylim=c(0,max(c(max(out$fx),max(hist(x,plot=FALSE)$density)))))
      lines(out$x,out$fx,lty=1,lwd=2)
   }
   return(x)
}
```

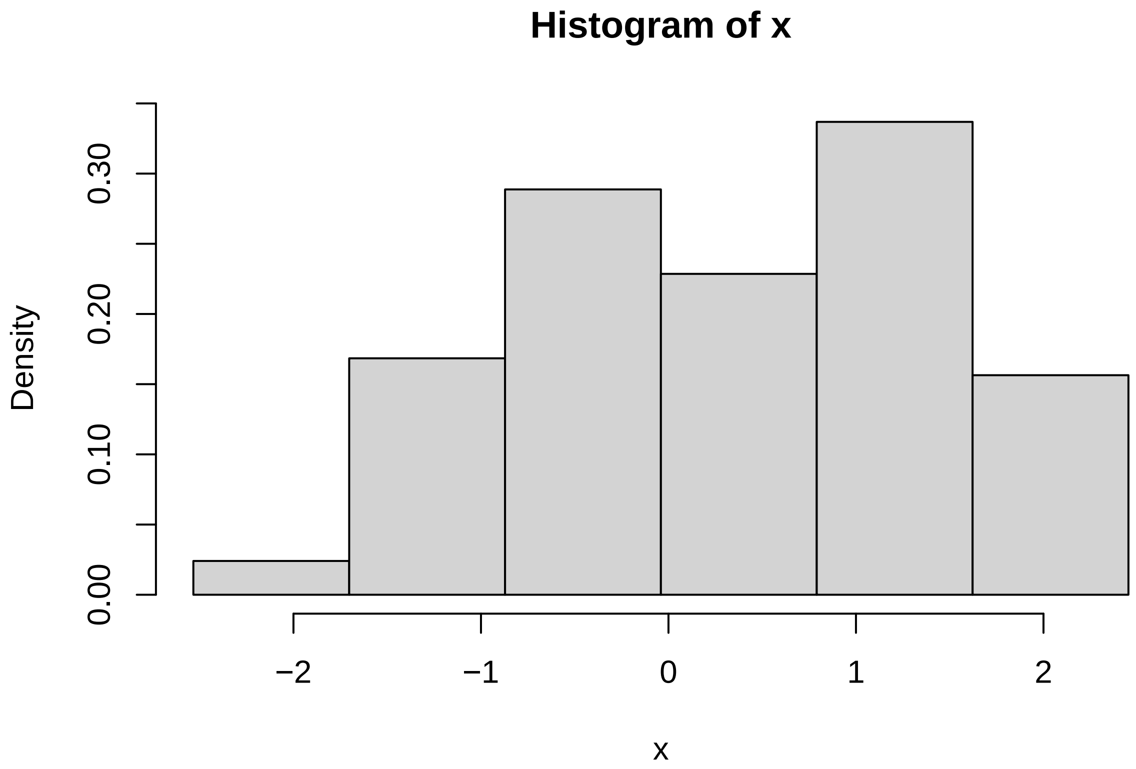
```
set.seed(123)
n <- 100
mu <- c(0,3/2)
sigma <- c(1,1/3)
alpha <- c(3/4,1/4)
x <- sim.mixt(n=n, k=2, mu=mu, sigma=sigma, alpha=alpha, gr=T)
points(x,0*x,pch="|")
```



```
b_scott <- function(X){
  return(3.49 * sd(X) * length(X)**(-1/3))
}

A <- min(x)-.05*diff(range(x))
Z <- max(x)+.05*diff(range(x))

b <- b_max_log_lik(b_set, x)
hx <- hist(x, breaks=seq(A, Z+b, by=b), plot=F)
plot(hx, freq = FALSE)
```



```
b_s <- b_scott(x)
hx_s <- hist(x, breaks=seq(A, Z+b_s, by=b_s), plot=F)
plot(hx_s, freq = FALSE)
```



Kernel density estimator

8.Consider the vector x of data you have generated before from the mixture of two normals. Use the relationship

$$\hat{f}_{h,(-i)}(x_i) = \frac{n}{n-1}\left(\hat{f}_h(x_i) - \frac{K(0)}{nh}\right)$$

to select the value of **h** maximizing the leave-one-out log-likelihood function, and plot the corresponding kernel density estimator. NOTE: The following sentences converts the kernel density estimator obtained with the function *density* into a function that can be evaluated at any point of R or at a vector of real numbers:

```
kx <- density(x)
kx_f <- approxfun(x=kx$x, y=kx$y, method = 'linear', rule=2)
```