Density Estimation

Bandwidht choice by leave-one-out maximum likelihood

Biel Caballero, Menzenbach Svenja and Reyes Illescas Kleber Enrique

2023-09-25

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:

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

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

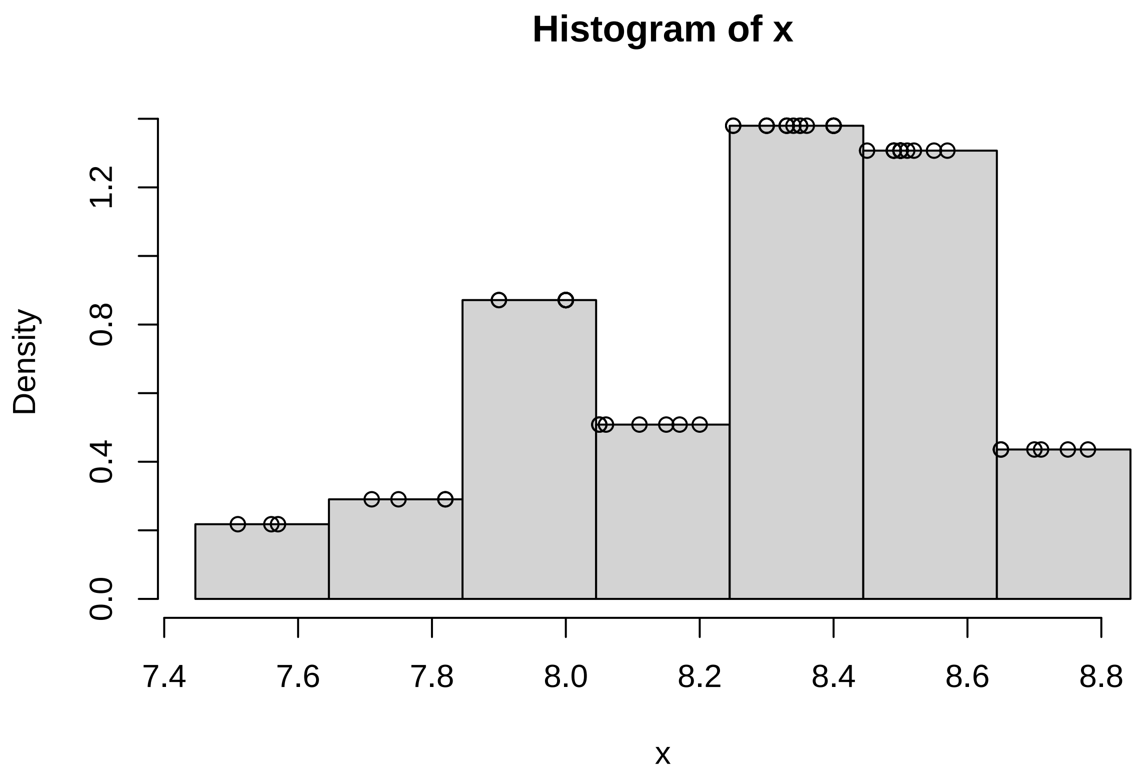
$$\hat{f}_{hist,(-i)}(x_i) = \frac{n}{n-1}\hat{f}_{hist}(x_i) - \frac{1}{(n-1)b}$$

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

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))
```



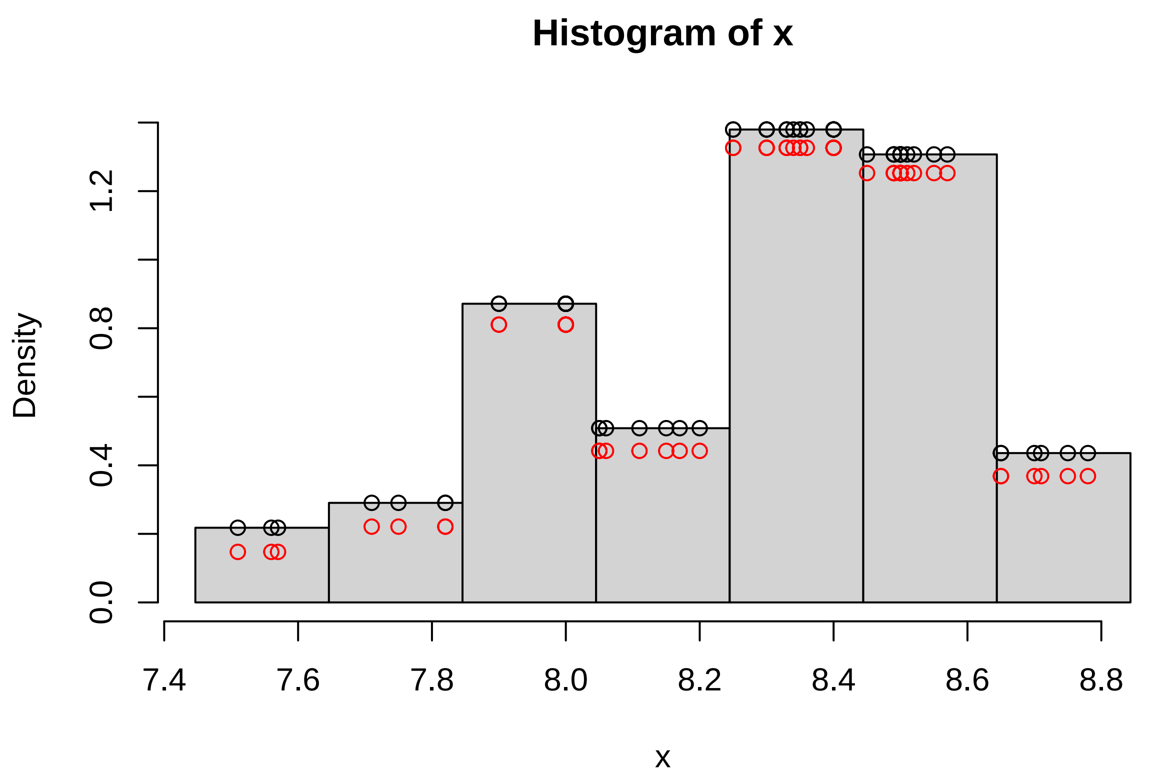
3. Use the formula you have found before relating $\hat{f}_{hist}(x_i)$ and $\hat{f}_{hist,(-i)}(x_i)$ to compute $\hat{f}_{hist,(-i)}(x), i = 1, ..., n,$. Then, add the points $(x_i, \hat{f}_{hist,(-i)}(x_i)), i = 1, ..., n,$ to the previous plot.

   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
hx_f2<-(length(x)/(length(x)-1)* hx_f(x))- 1/((length(x)-1)*(hx$breaks[2]-hx$breaks[1]))

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] -16.58432
```

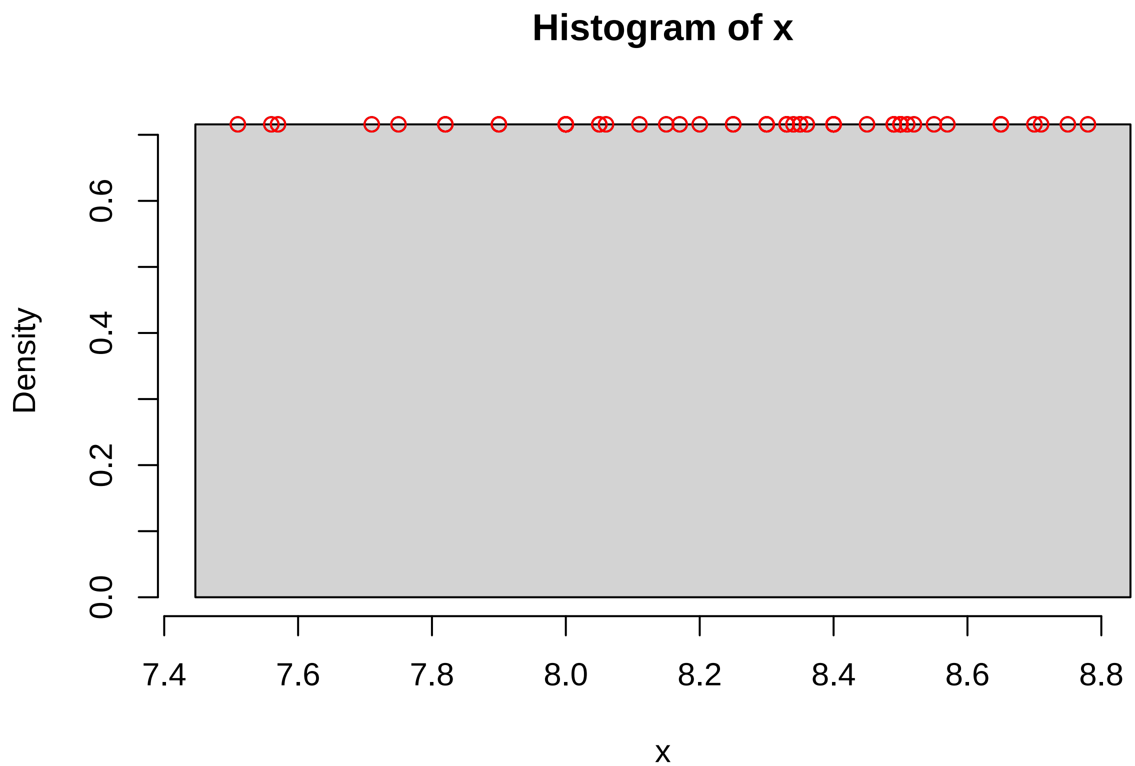
5. **Choosing *nbr* by leave-one-out Cross Validation (looCV)**. Consider now the set *seq(1,15)* as possible values for *nbr*, the number of intervals of the histogram. For each of them compute the leave-one-out log-likelihood function (*looCv_log_lik*) fir the corresponding histogram. Then plot the 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()

for (nbr in c(1:15)){
  #A <- min(hx_f2)-.05*diff(range(hx_f2))
  #Z <- max(hx_f2)+.05*diff(range(hx_f2))
  hx_i <- hist(x,breaks=seq(A,Z,length=nbr+1),freq=F, plot = FALSE)
  hx_f_i <- stepfun(hx_i$breaks,c(0,hx_i$density,0))
  n <- length(x)
  b <- hx_i$breaks[2]-hx_i$breaks[1]
  hx_f2_i <- n/(n-1)*hx_f_i(x) - 1/((n-1)*b)
  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))
  log_liks <- append(log_liks, looCV_log_lik)
}
```

```
## Warning in hist.default(x, breaks = seq(A, Z, length = nbr + 1), freq = F, :
## argument 'freq' is not made use of
```

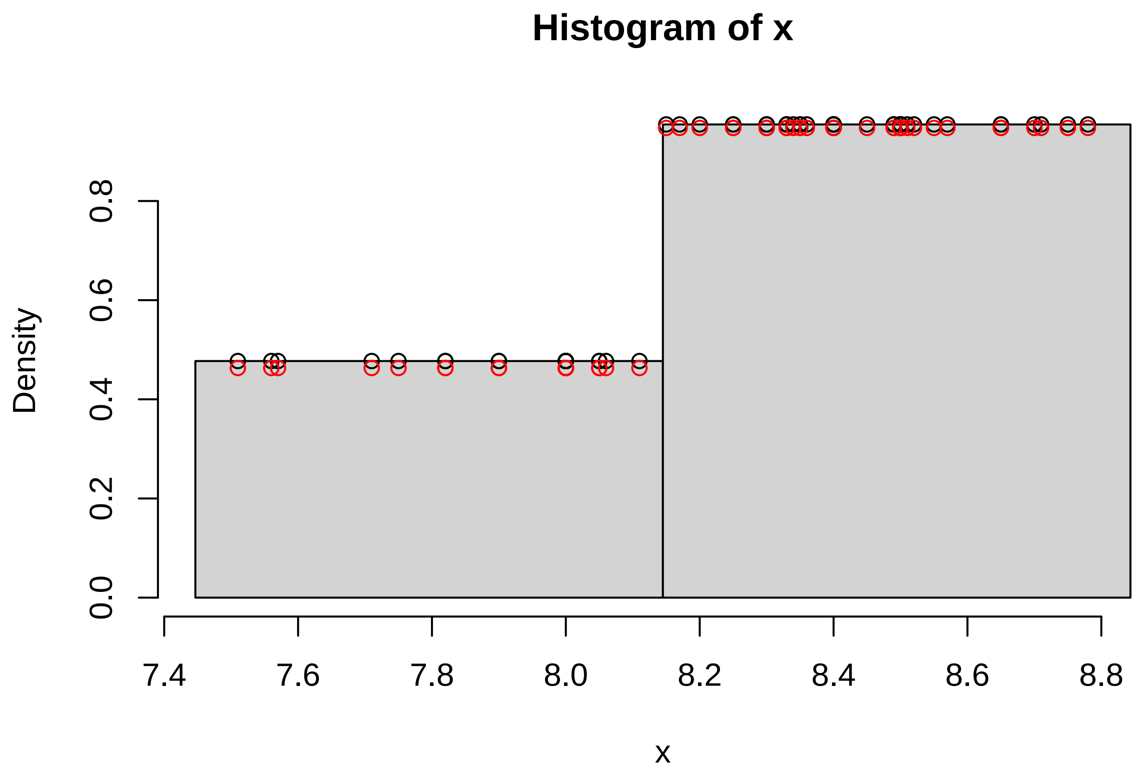
```
## [1] 0.7158196
```

```
## Warning in hist.default(x, breaks = seq(A, Z, length = nbr + 1), freq = F, :
## argument 'freq' is not made use of
```

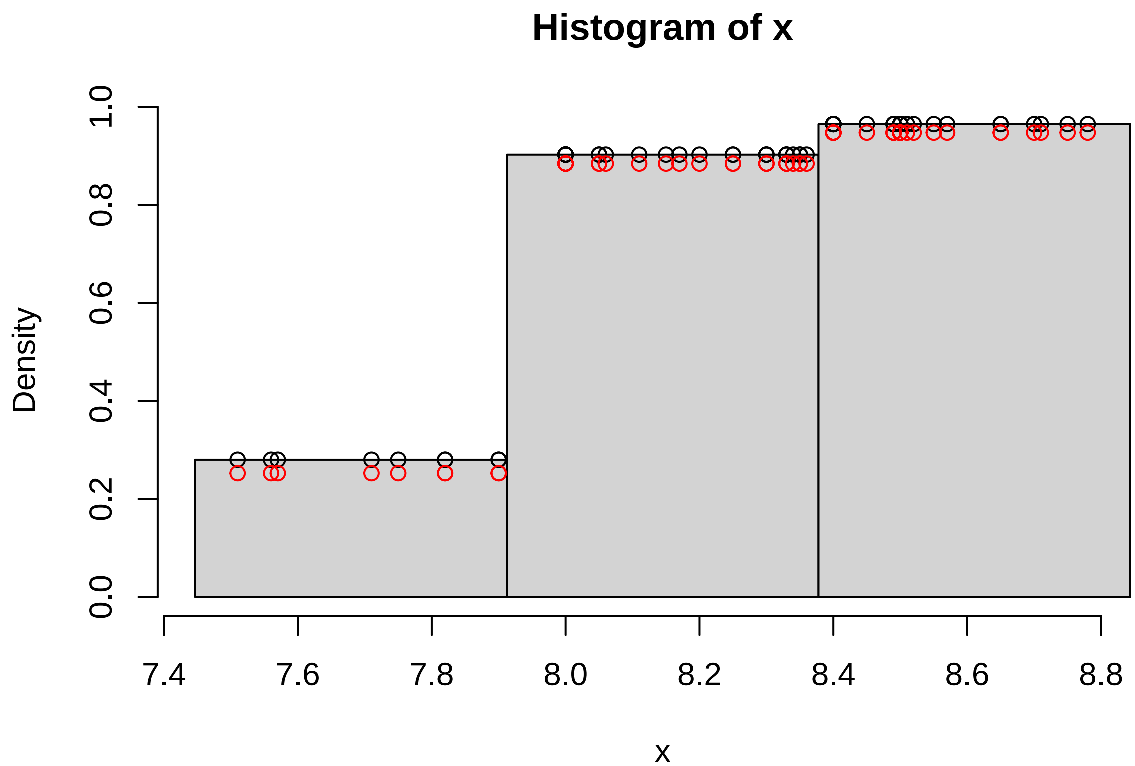



```
## [1] 0.4631774
```

```
## Warning in hist.default(x, breaks = seq(A, Z, length = nbr + 1), freq = F, :
## argument 'freq' is not made use of
```

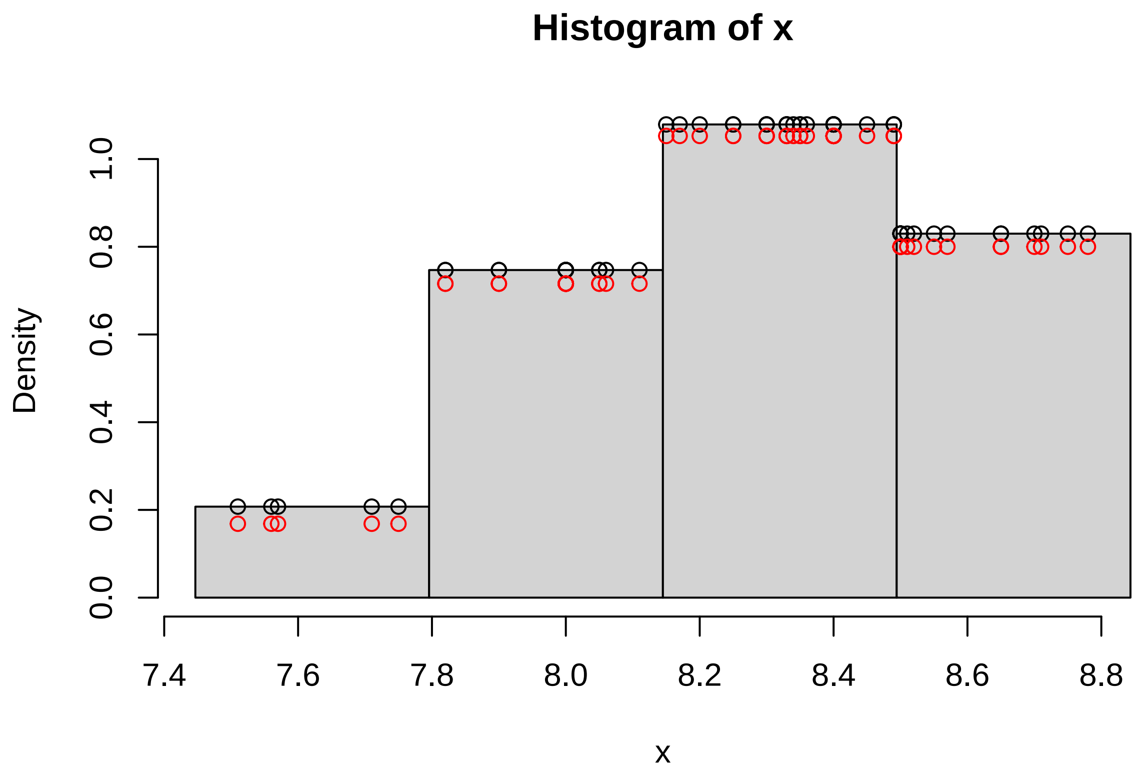



```
## [1] 0.2526422

## Warning in hist.default(x, breaks = seq(A, Z, length = nbr + 1), freq = F, :
## argument 'freq' is not made use of
```



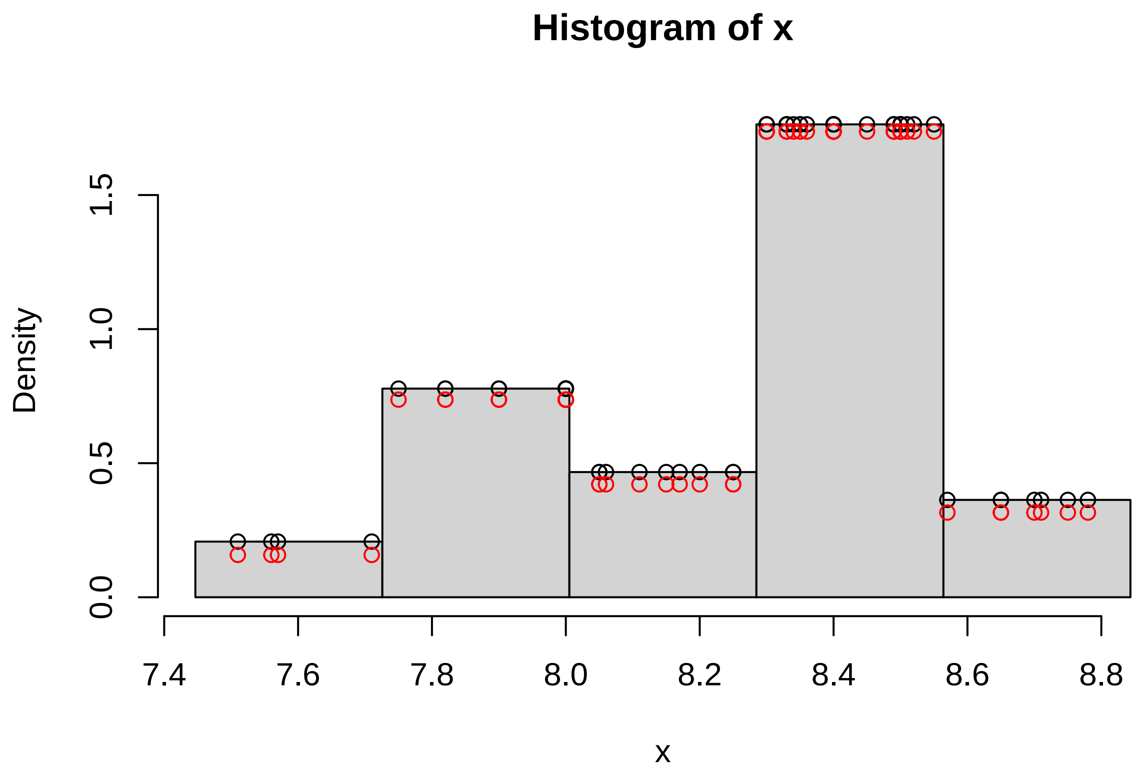

```
## [1] 0.1684281
```

```
## Warning in hist.default(x, breaks = seq(A, Z, length = nbr + 1), freq = F, :
## argument 'freq' is not made use of
```



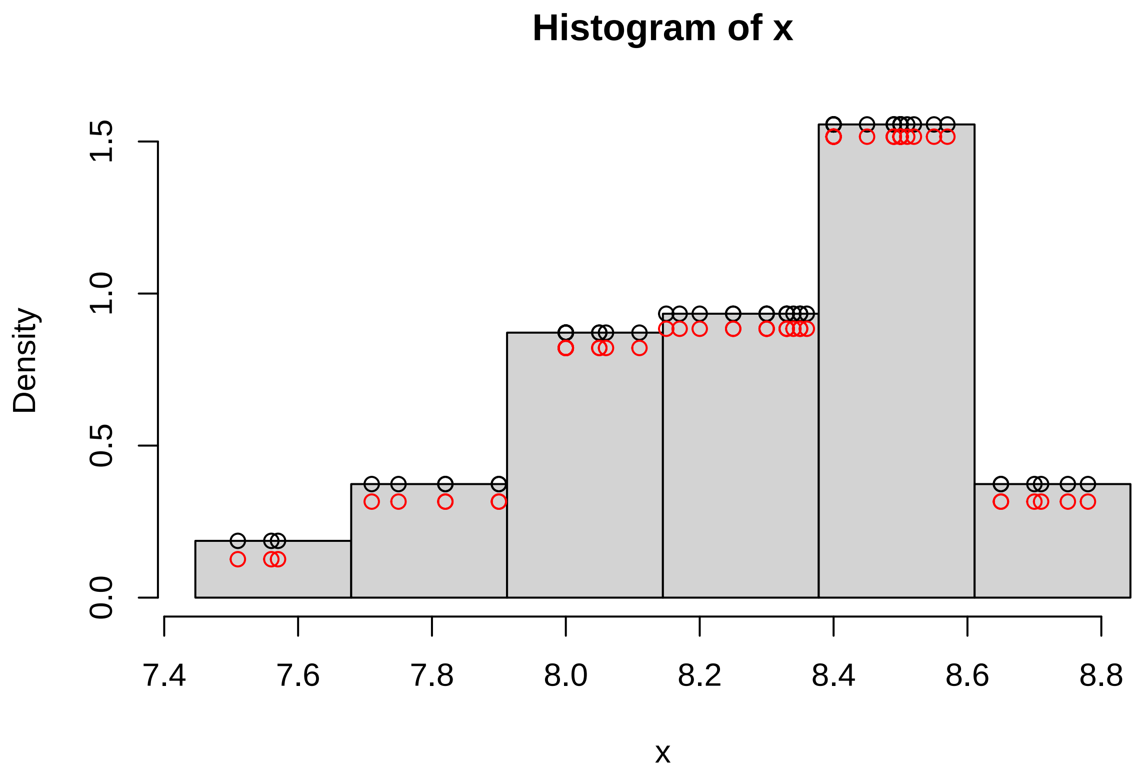

```
## [1] 0.1579014
```

```
## Warning in hist.default(x, breaks = seq(A, Z, length = nbr + 1), freq = F, :
## argument 'freq' is not made use of
```



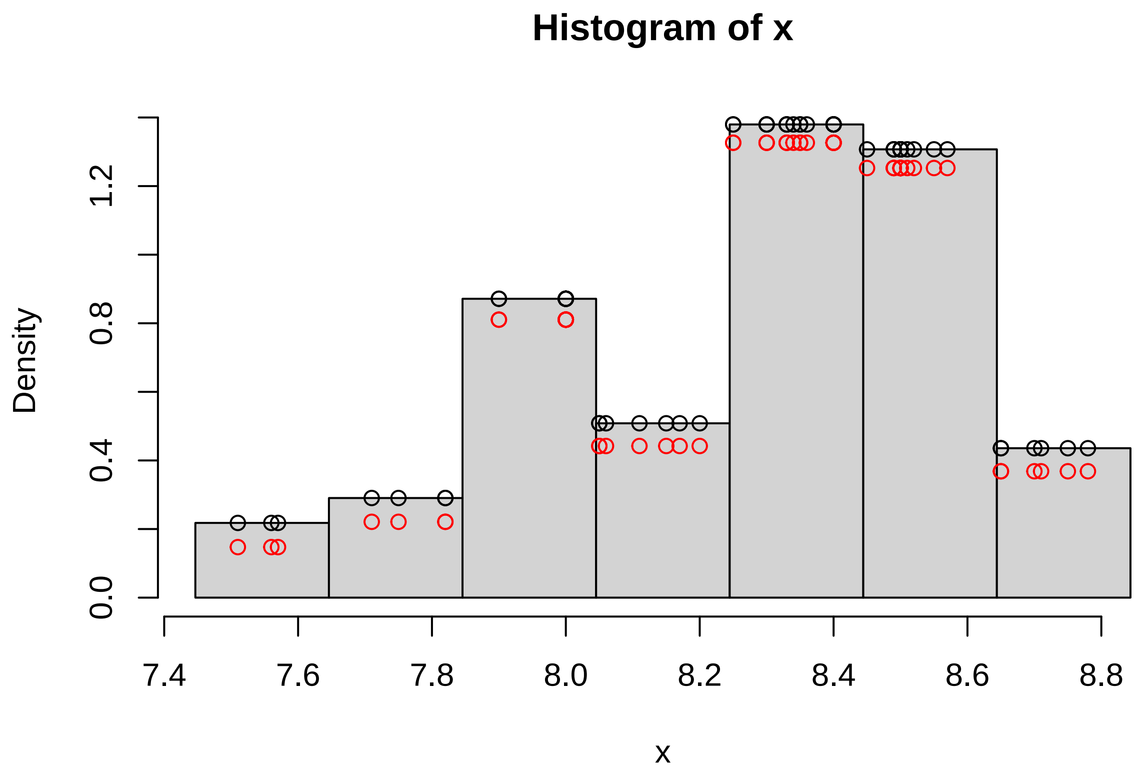

```
## [1] 0.1263211
```

```
## Warning in hist.default(x, breaks = seq(A, Z, length = nbr + 1), freq = F, :
## argument 'freq' is not made use of
```



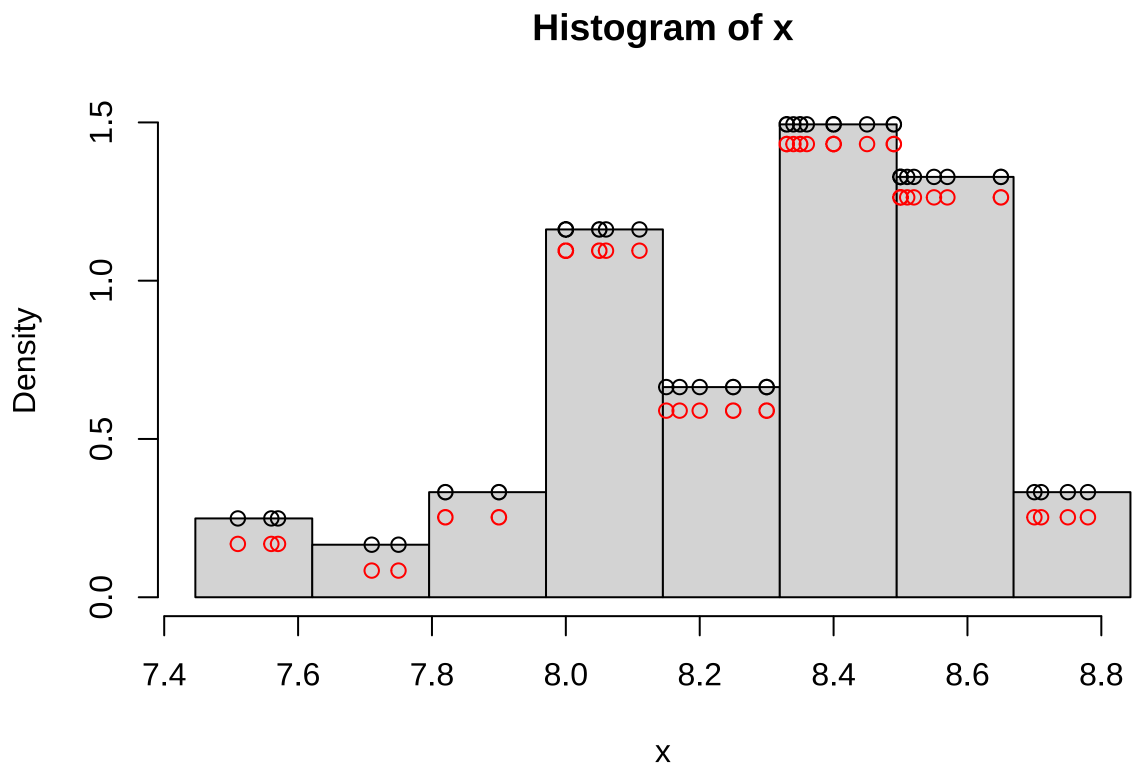

```
## [1] 0.1473746
```

```
## Warning in hist.default(x, breaks = seq(A, Z, length = nbr + 1), freq = F, :
## argument 'freq' is not made use of
```

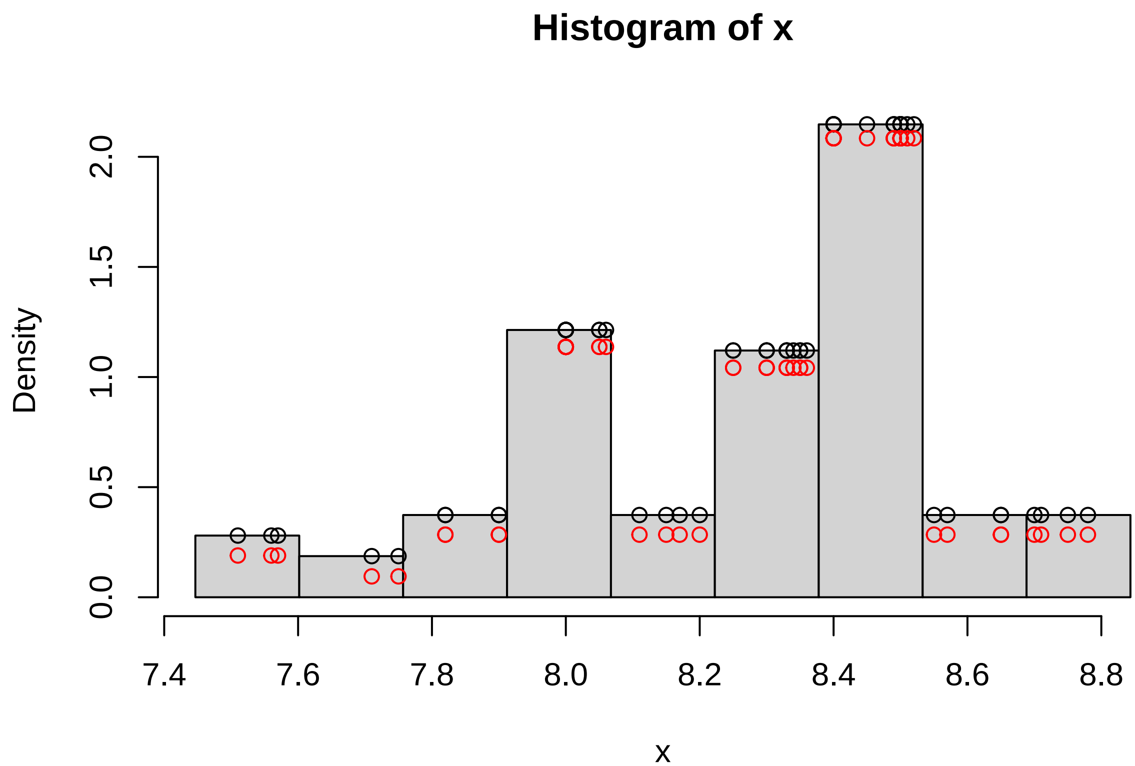



```
## [1] 0.08421407
```

```
## Warning in hist.default(x, breaks = seq(A, Z, length = nbr + 1), freq = F, :
## argument 'freq' is not made use of
```

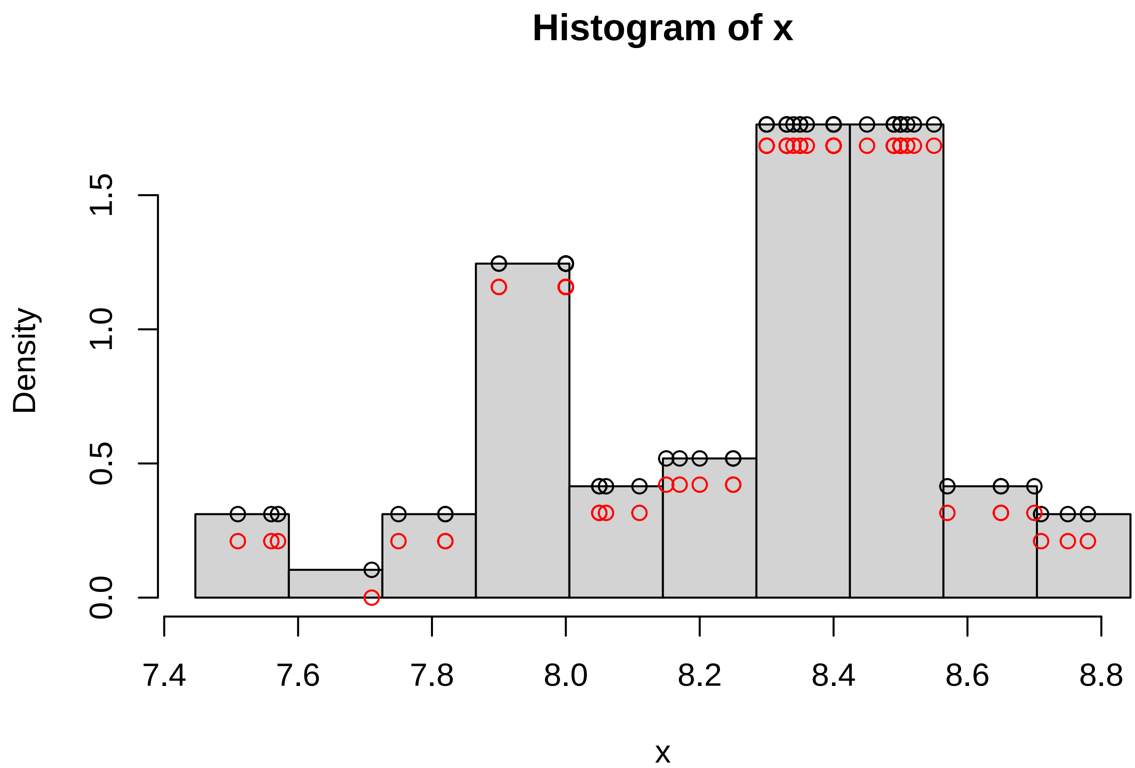



```
## [1] 0.09474083

## Warning in hist.default(x, breaks = seq(A, Z, length = nbr + 1), freq = F, :
## argument 'freq' is not made use of
```

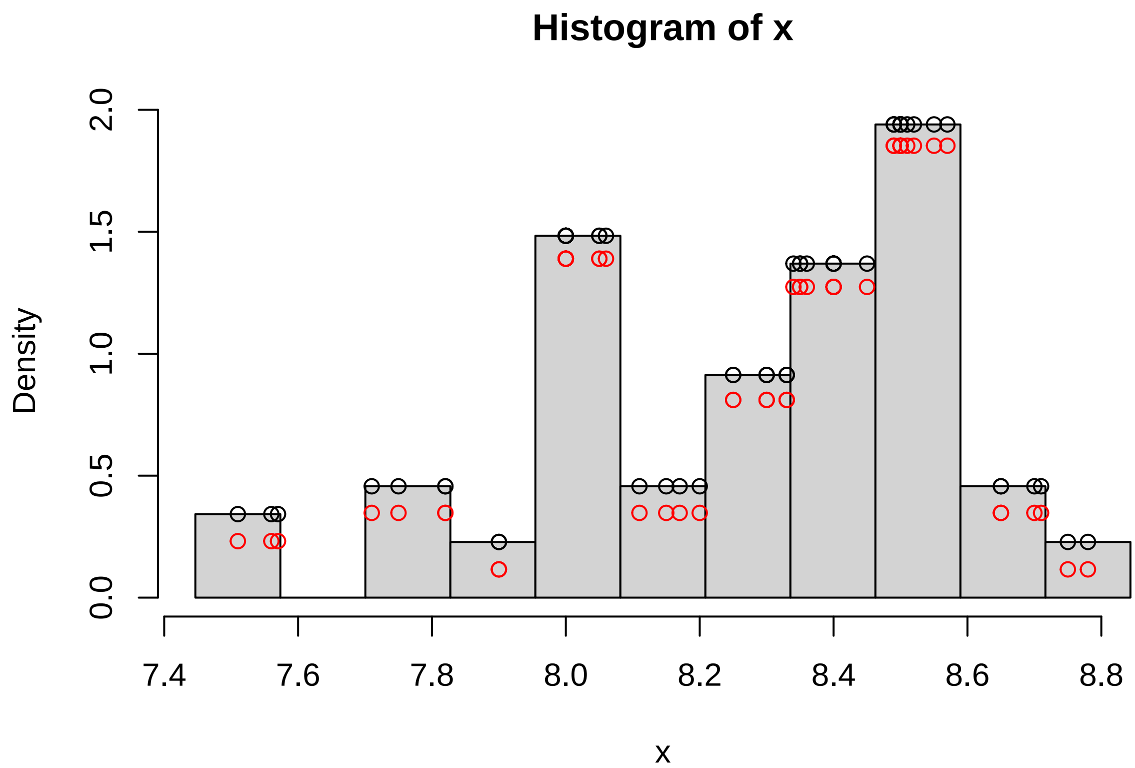



```
## [1] 6.661338e-16
```

```
## Warning in hist.default(x, breaks = seq(A, Z, length = nbr + 1), freq = F, :
## argument 'freq' is not made use of
```

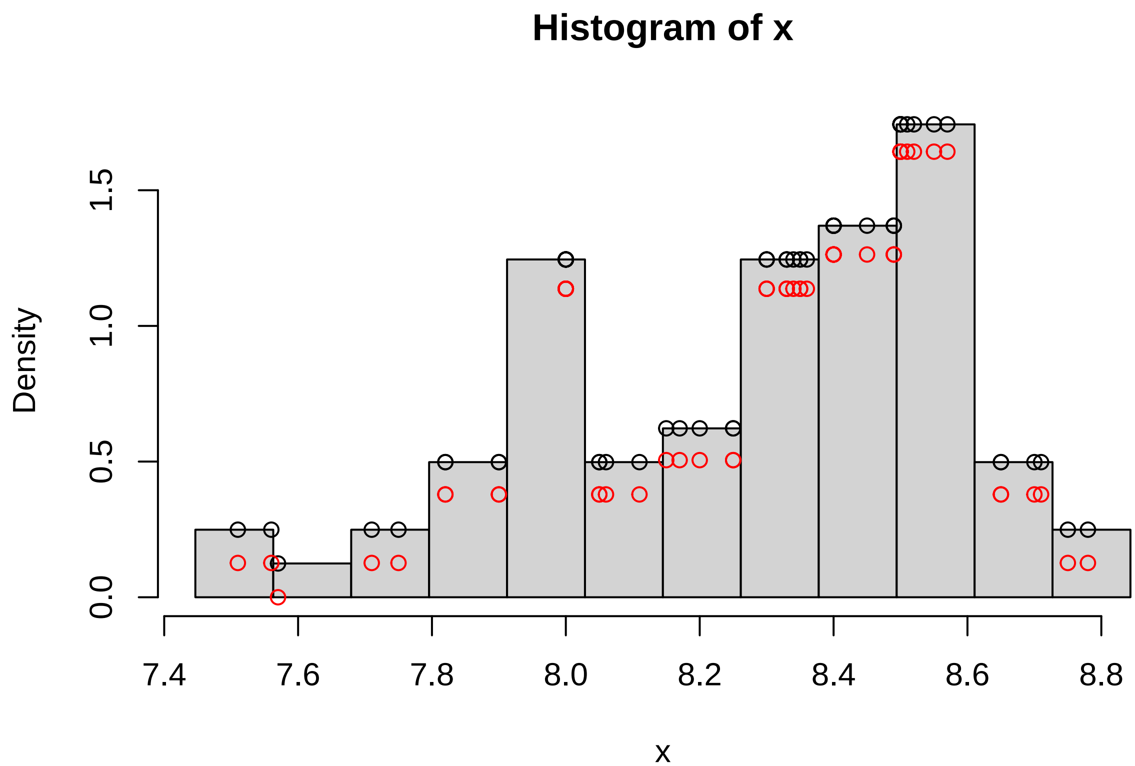



```
## [1] 0.1157943

## Warning in hist.default(x, breaks = seq(A, Z, length = nbr + 1), freq = F, :
## argument 'freq' is not made use of
```

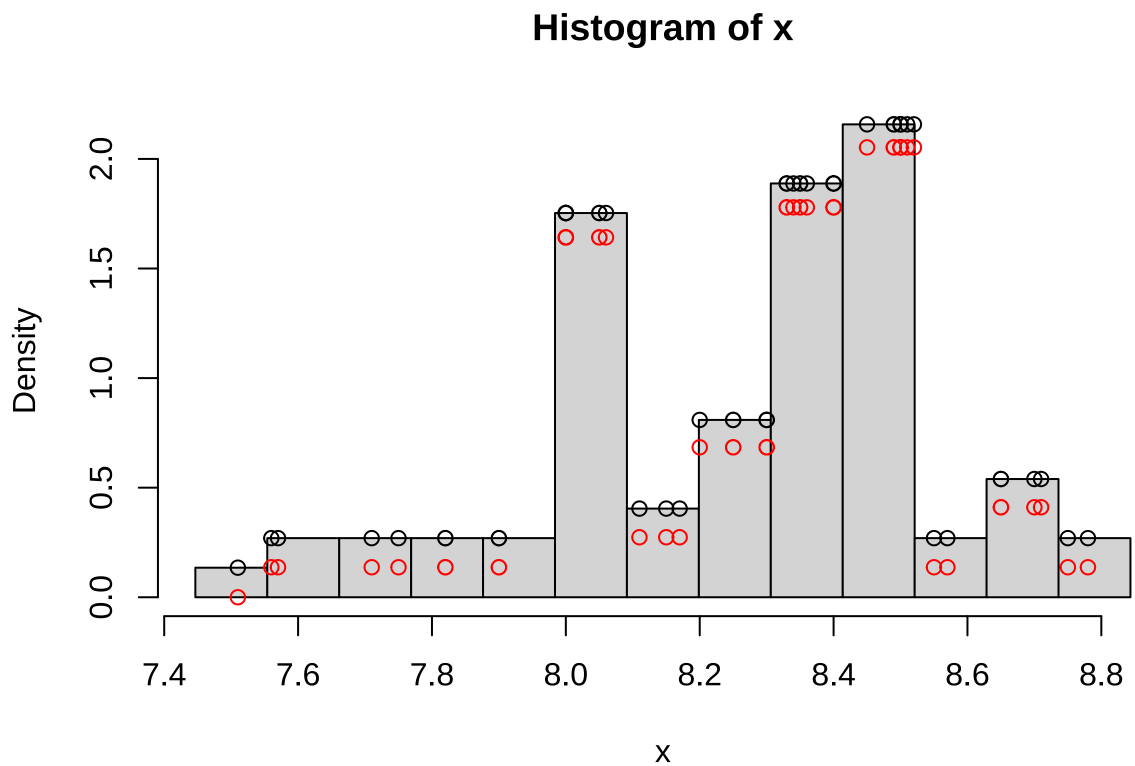



```
## [1] 9.714451e-16
```

```
## Warning in hist.default(x, breaks = seq(A, Z, length = nbr + 1), freq = F, :
## argument 'freq' is not made use of
```

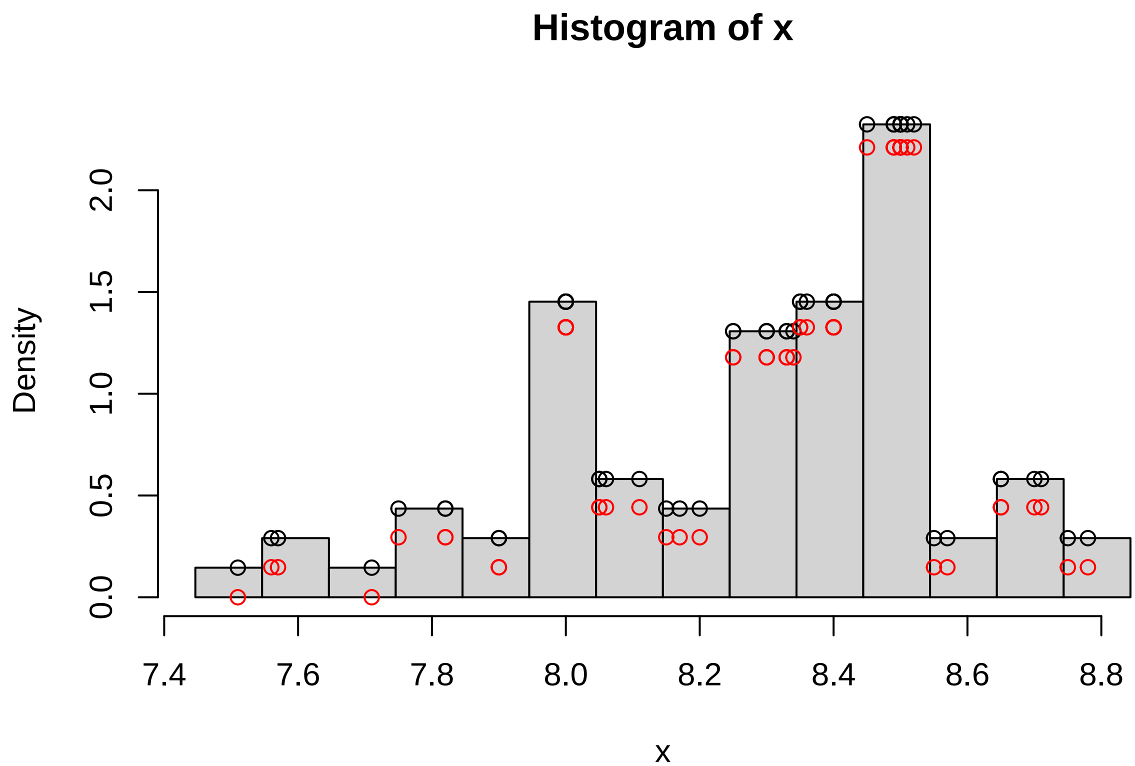



```
## [1] -2.775558e-17

## Warning in log(hx_f2_i): Se han producido NaNs

## Warning in log(hx_f2_i): argument 'freq' is not made use of
```



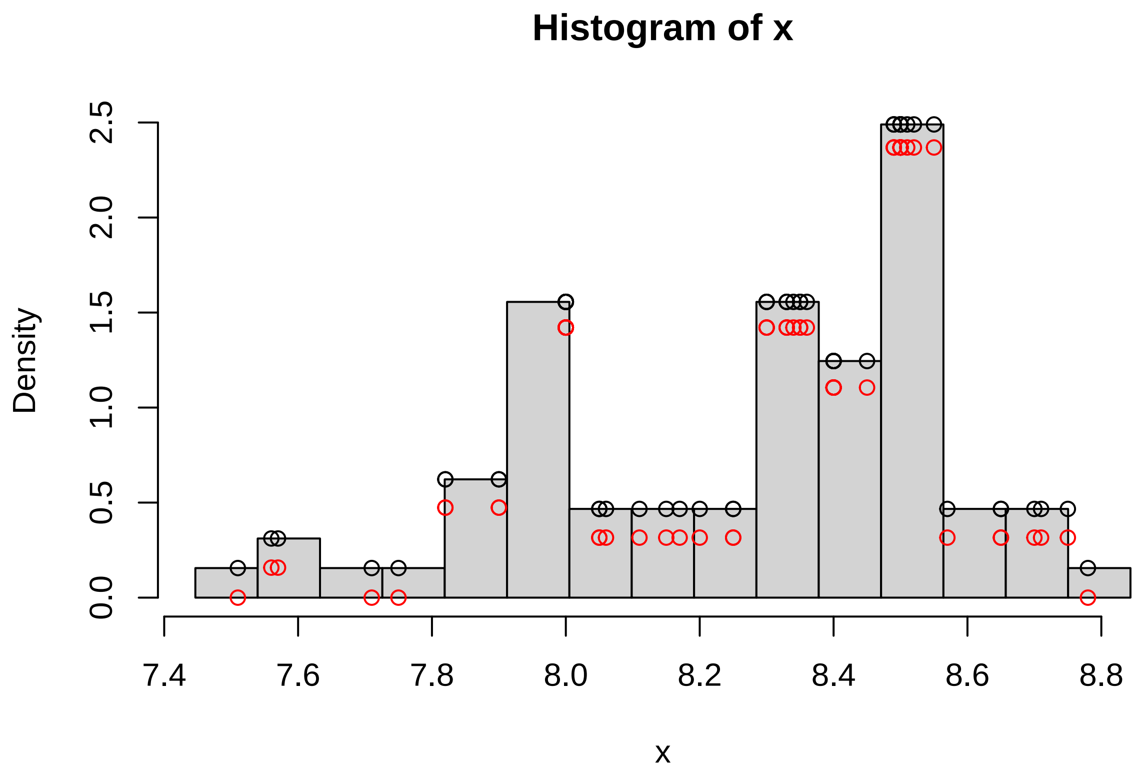

```
## [1] 0
```

```
## Warning in hist.default(x, breaks = seq(A, Z, length = nbr + 1), freq = F, :
## argument 'freq' is not made use of
```

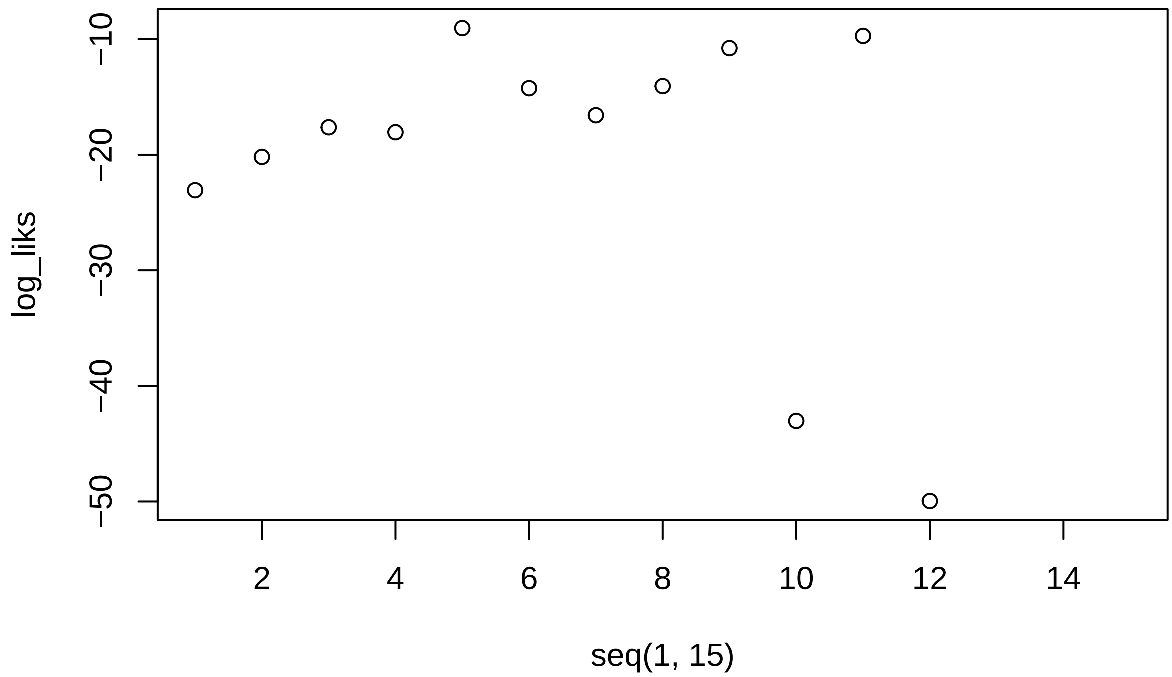



```
## [1] -1.498801e-15
```

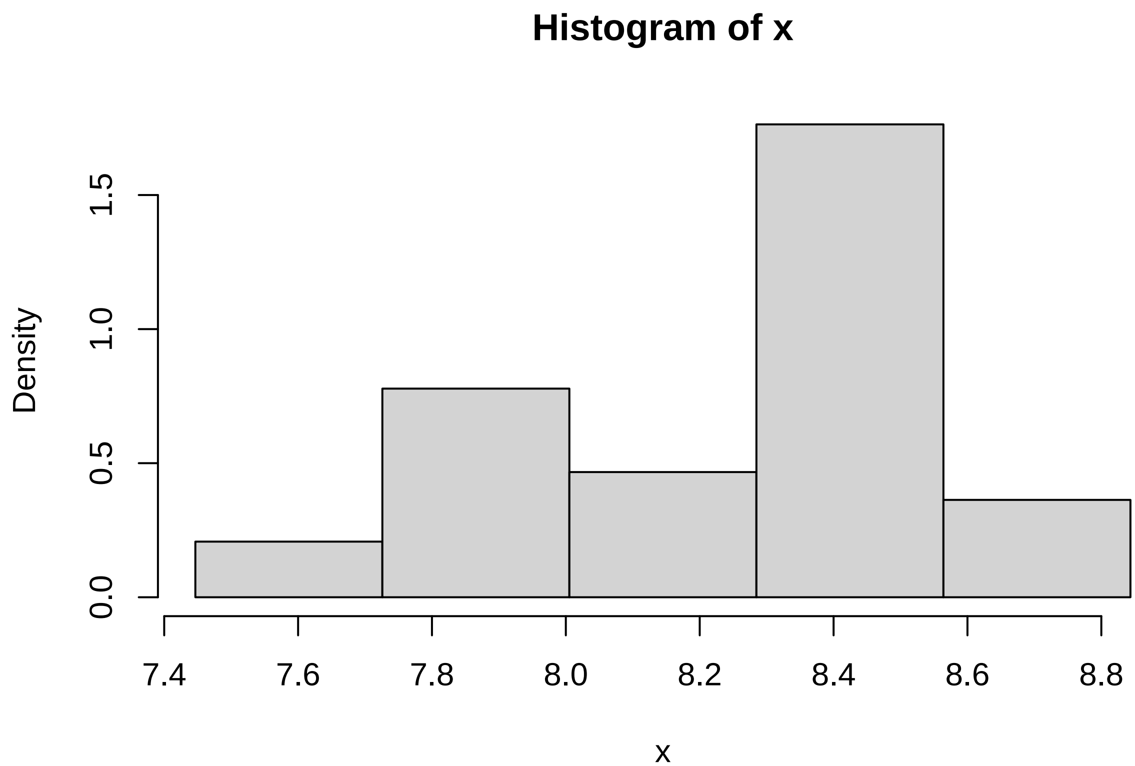
```
## Warning in log(hx_f2_i): Se han producido NaNs
```




```
plot(seq(1, 15), log_liks)
```



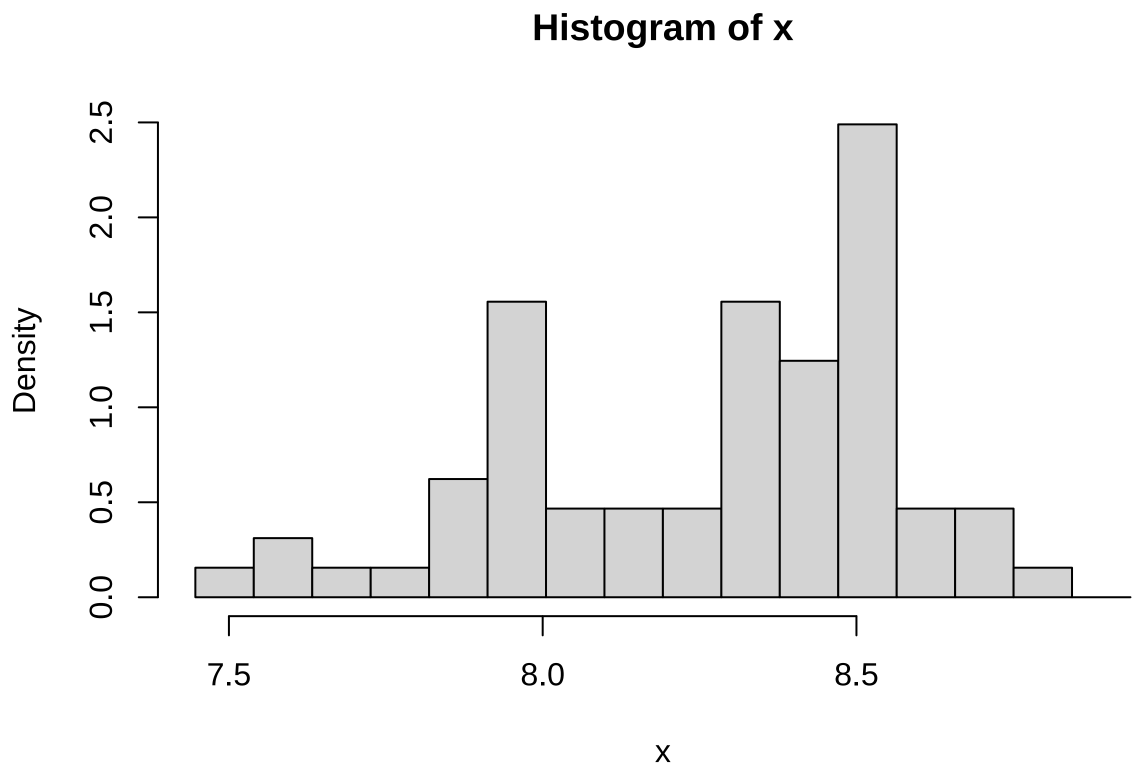

```
nbr_opt <- which.max(log_liks)
hist(x,breaks=seq(A,Z,length=nbr_opt+1),freq=F)
```



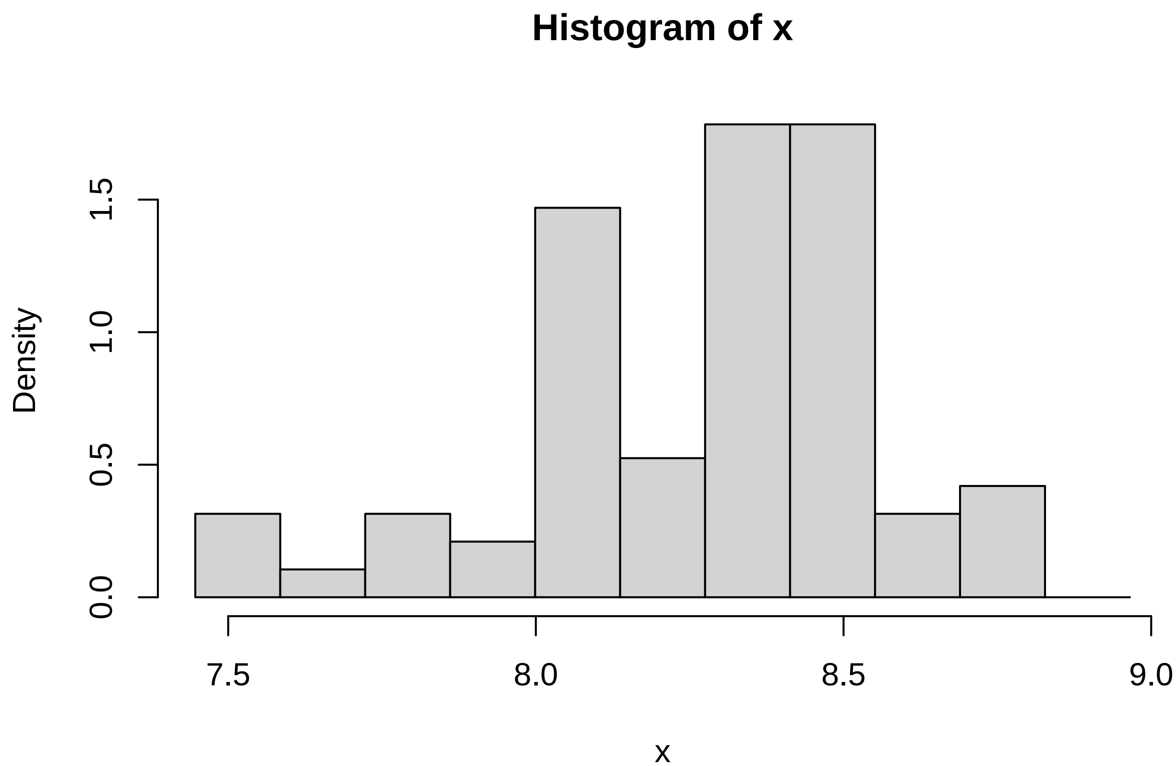

```
# TODO: - avoid production of NaNs,
#       - is it a problem that 'freq' is not used for some cases?
```

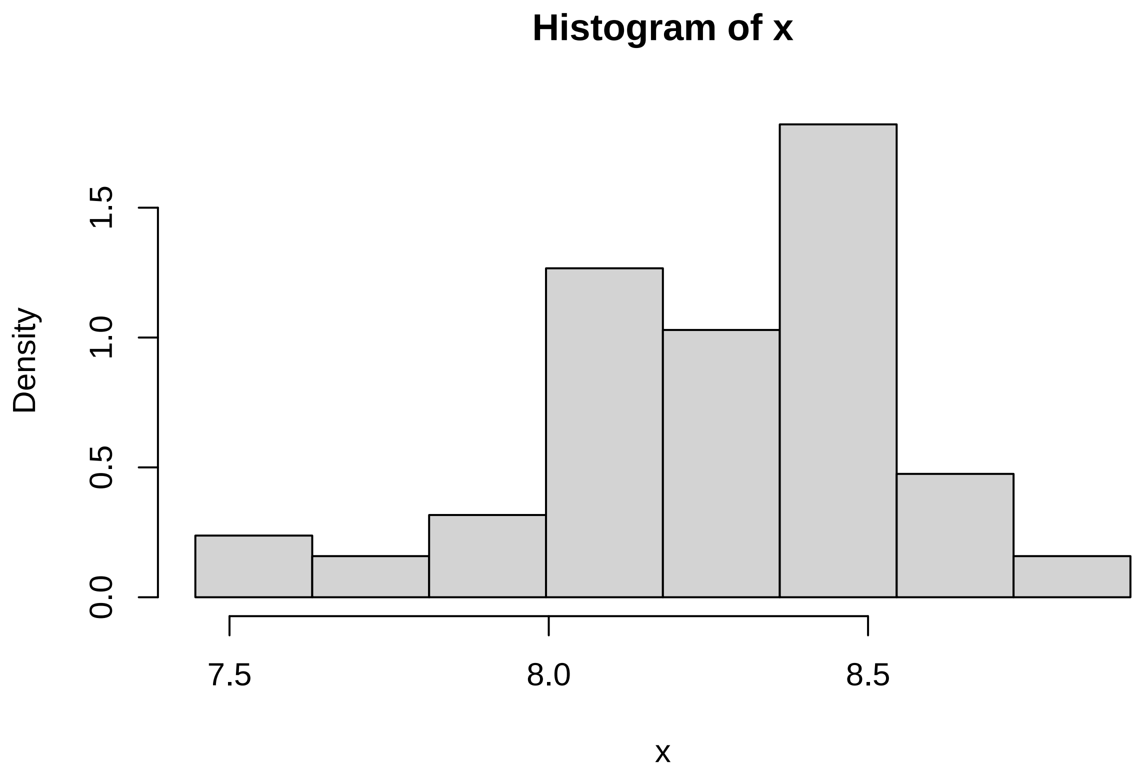
6. **Chossing b by looCV**. Let b be the common width of the bins of a histogram. Consider the set $seq((Z-A)/15,(Z-A)/1, length=30)$ as possible values for b. Select the value of b maximizing the leave-one-out log-likelihood function, and plot the corresponding histogram

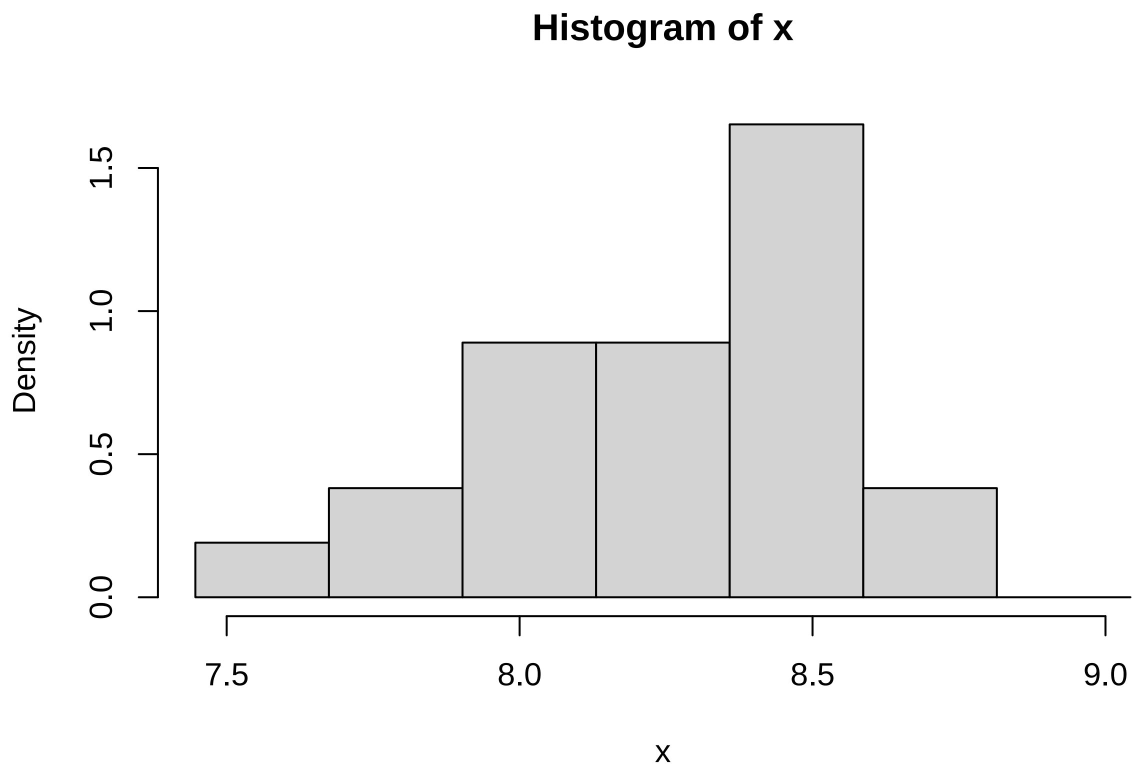
```
b_set <- seq((Z-A)/15, (Z-A), length=30)

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

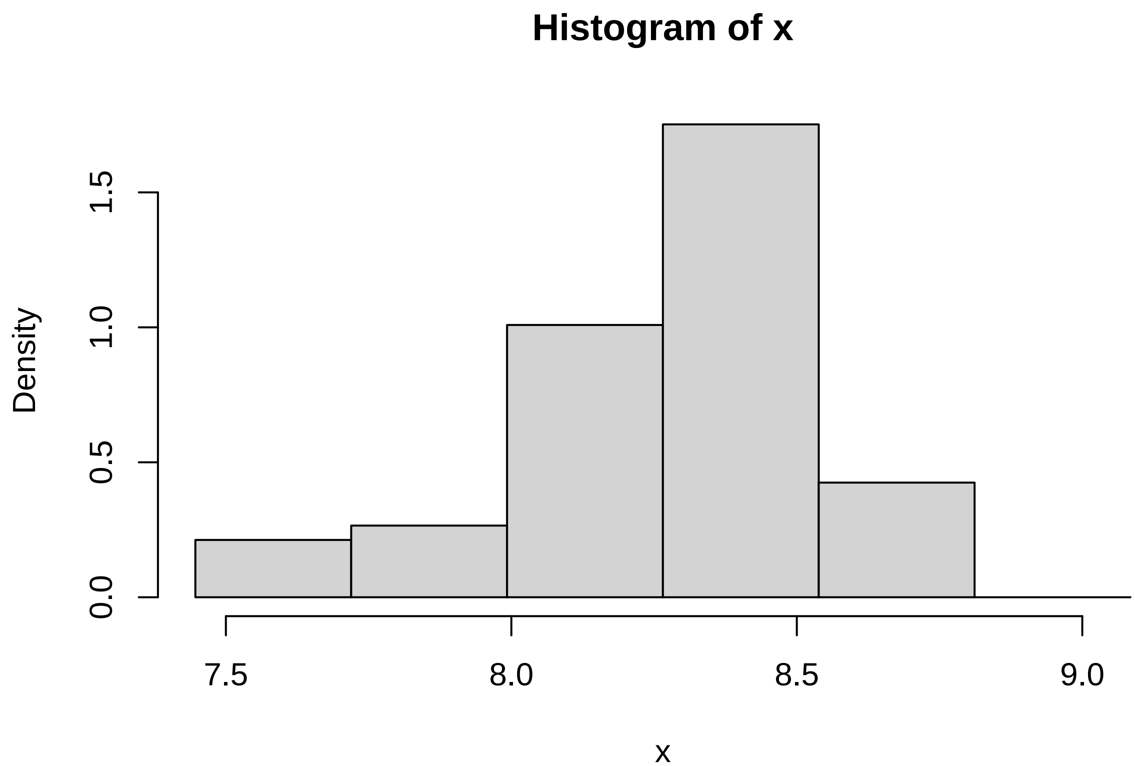


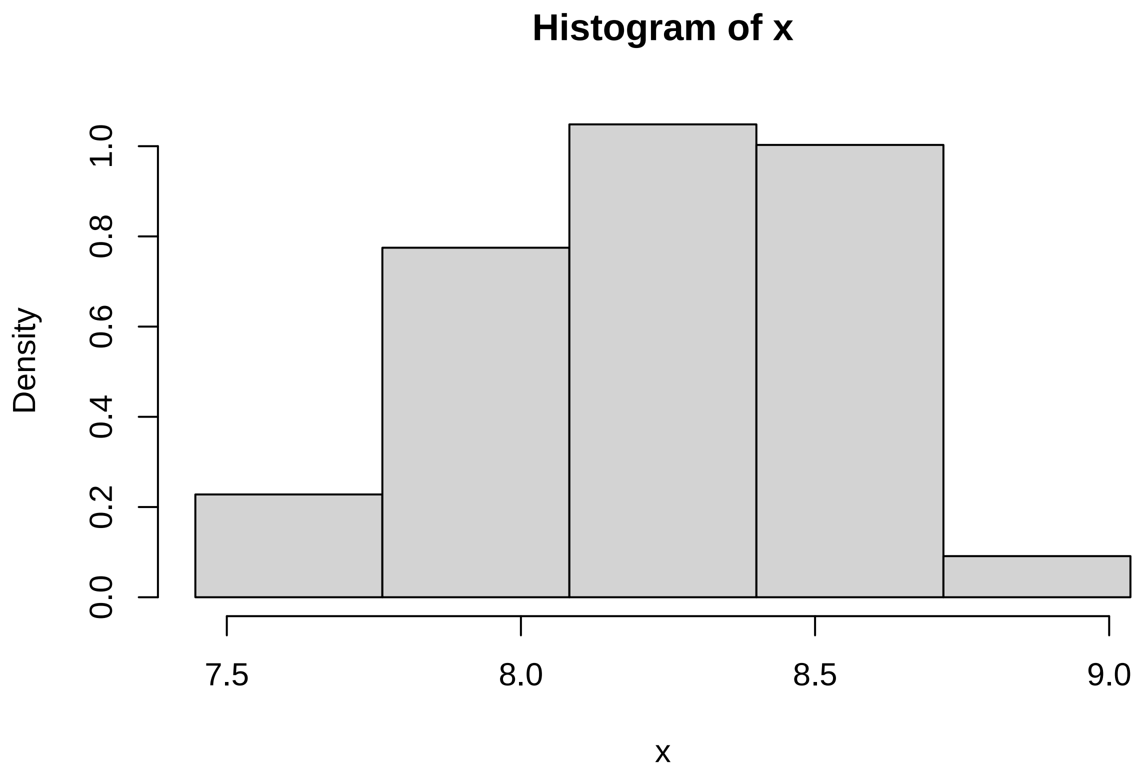
Histogram of x
Density
0.0
0.5
1.0
1.5
2.0
2.5
7.5
8.0
8.5
x

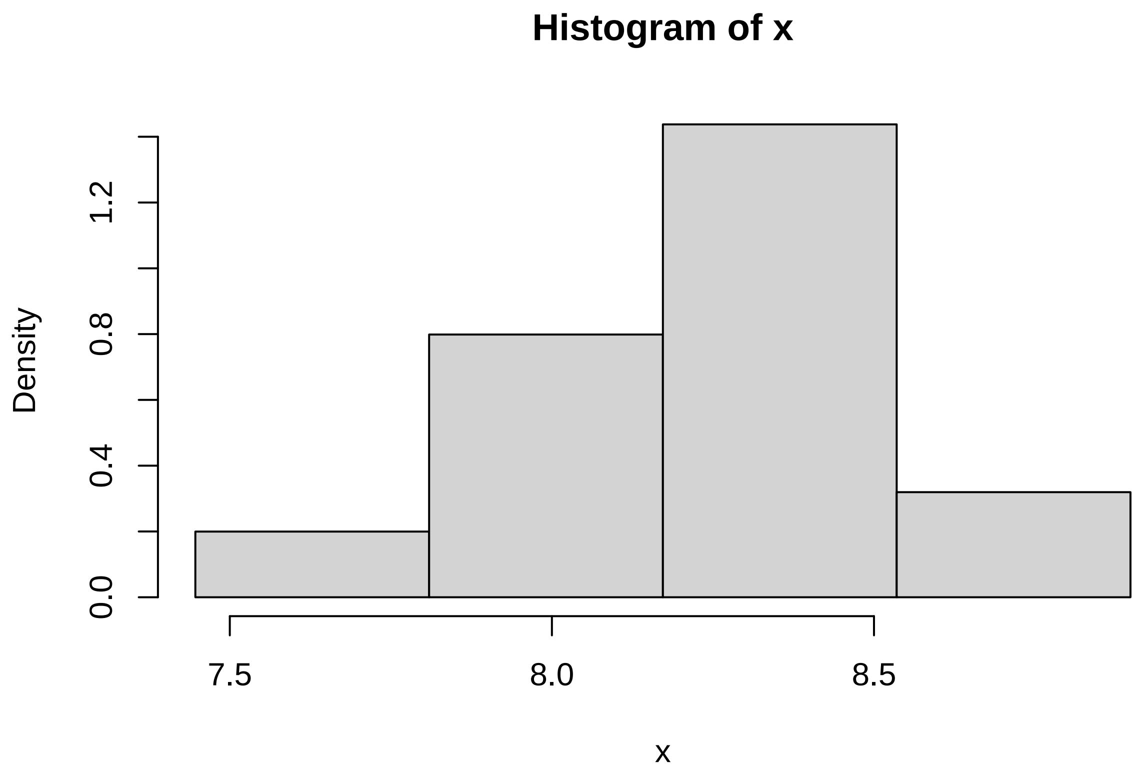

Histogram of x
Density
0.0
0.5
1.0
1.5
7.5
8.0
8.5
9.0
x

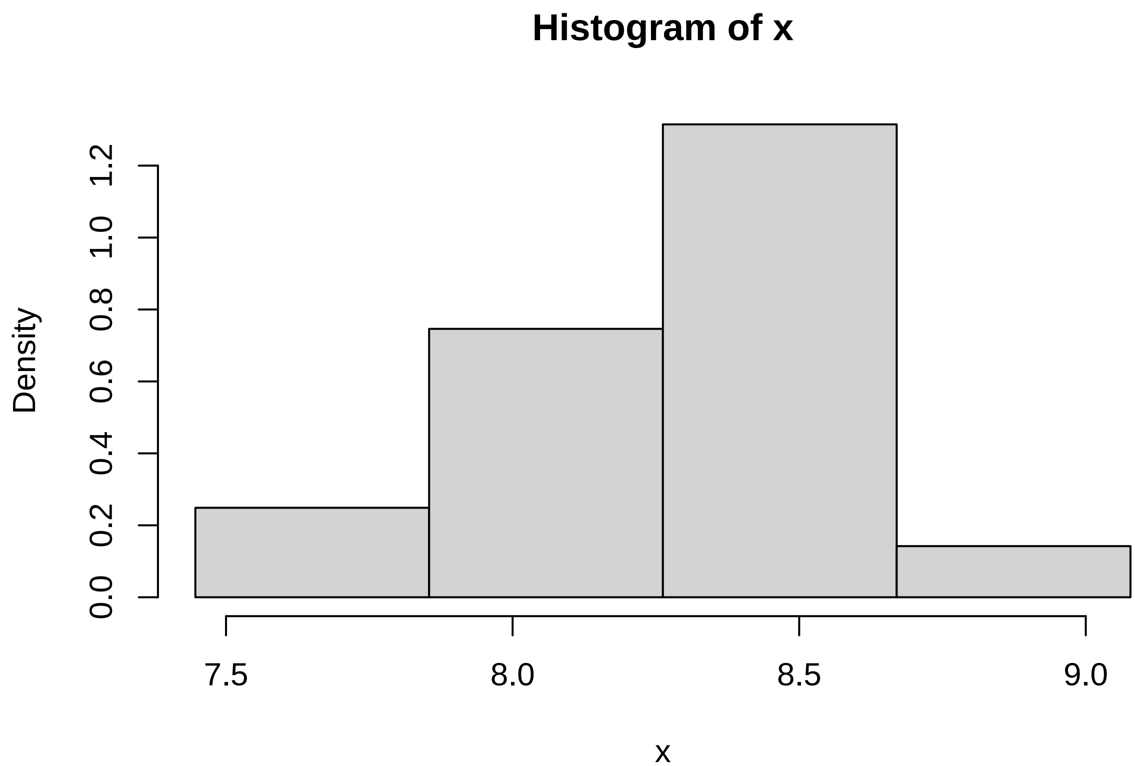

Histogram of x
Density
0.0
0.5
1.0
1.5
7.5
8.0
8.5
x

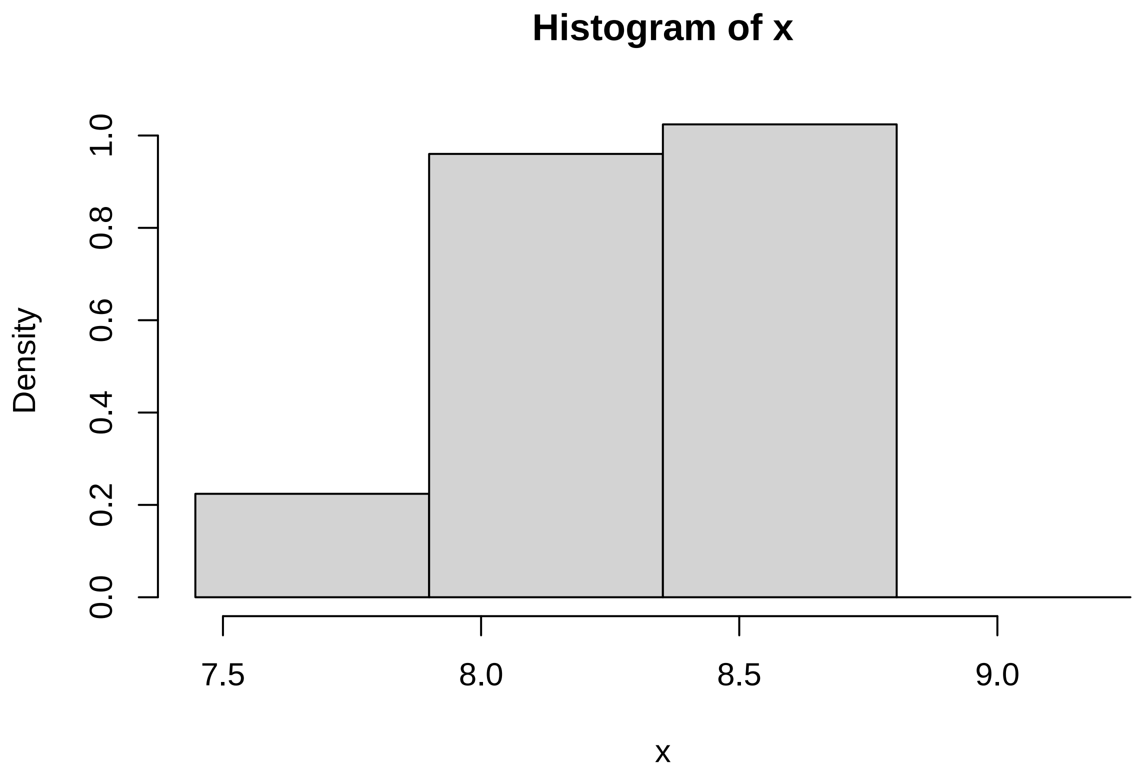

Histogram of x
Density
0.0
0.5
1.0
1.5
7.5
8.0
8.5
9.0
x

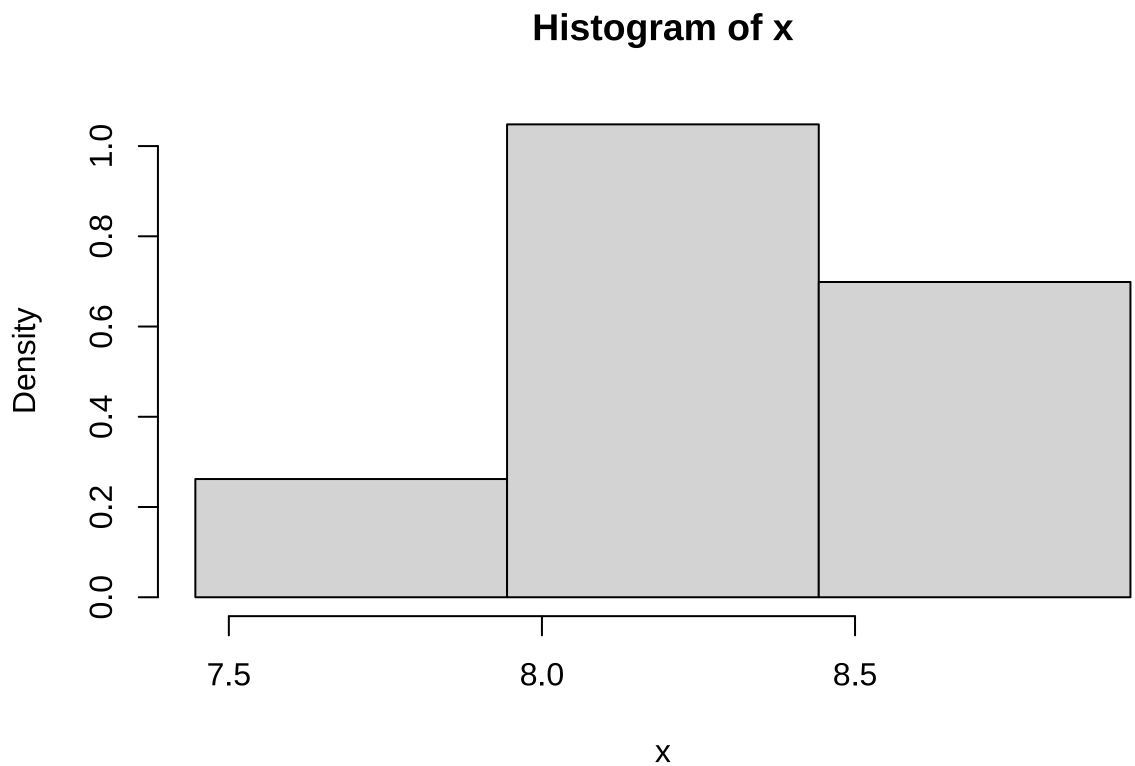

Histogram of x
Density
0.0
0.5
1.0
1.5
7.5
8.0
8.5
9.0
x

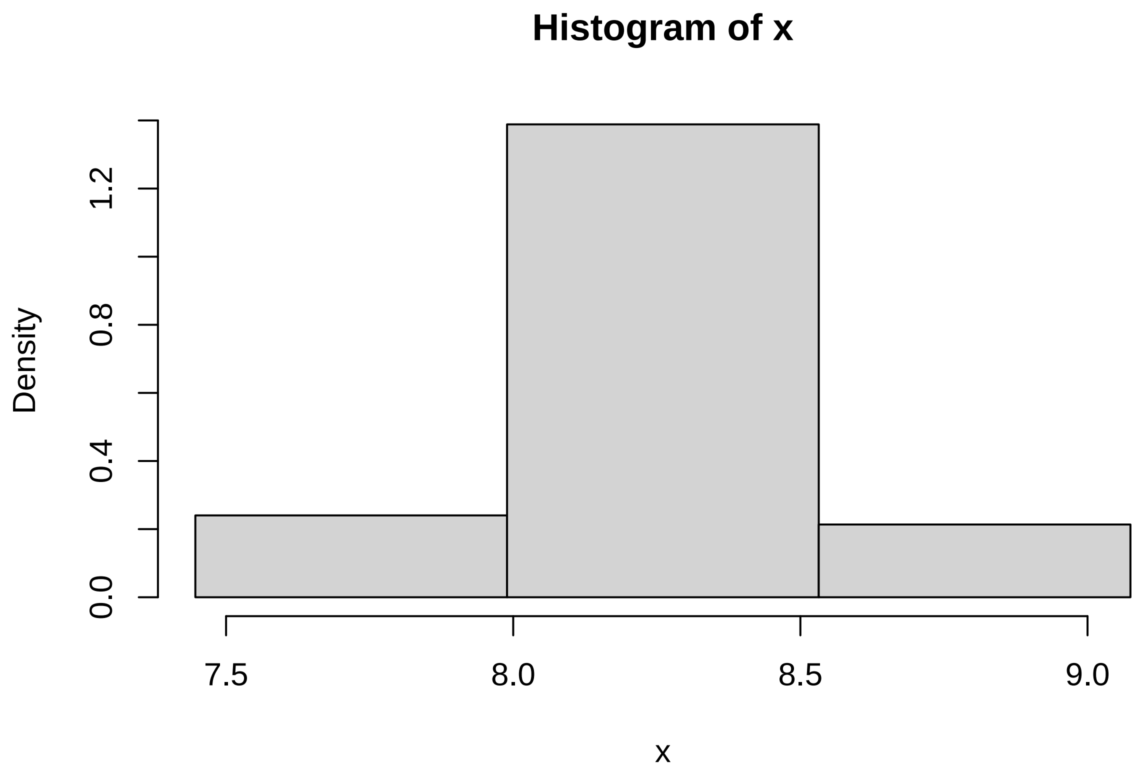

Histogram of x
Density
0.0
0.2
0.4
0.6
0.8
1.0
7.5
8.0
8.5
9.0
x

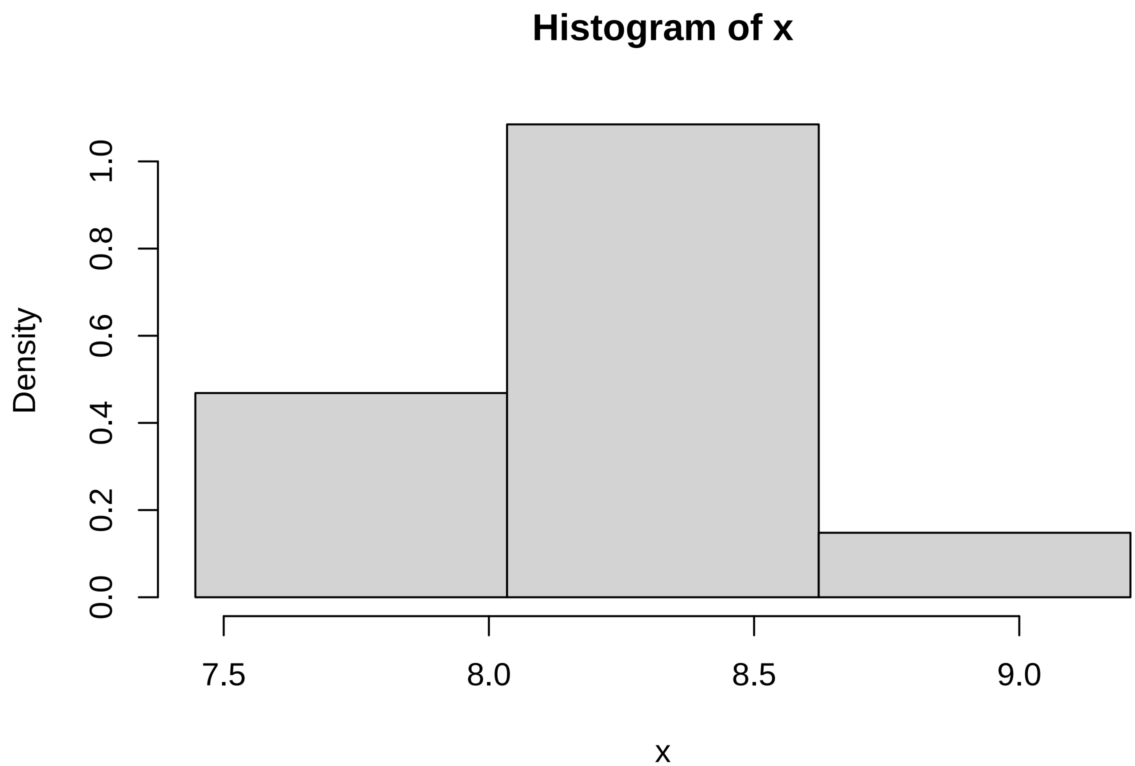

Histogram of x
Density
0.0
0.4
0.8
1.2
7.5
8.0
8.5
x

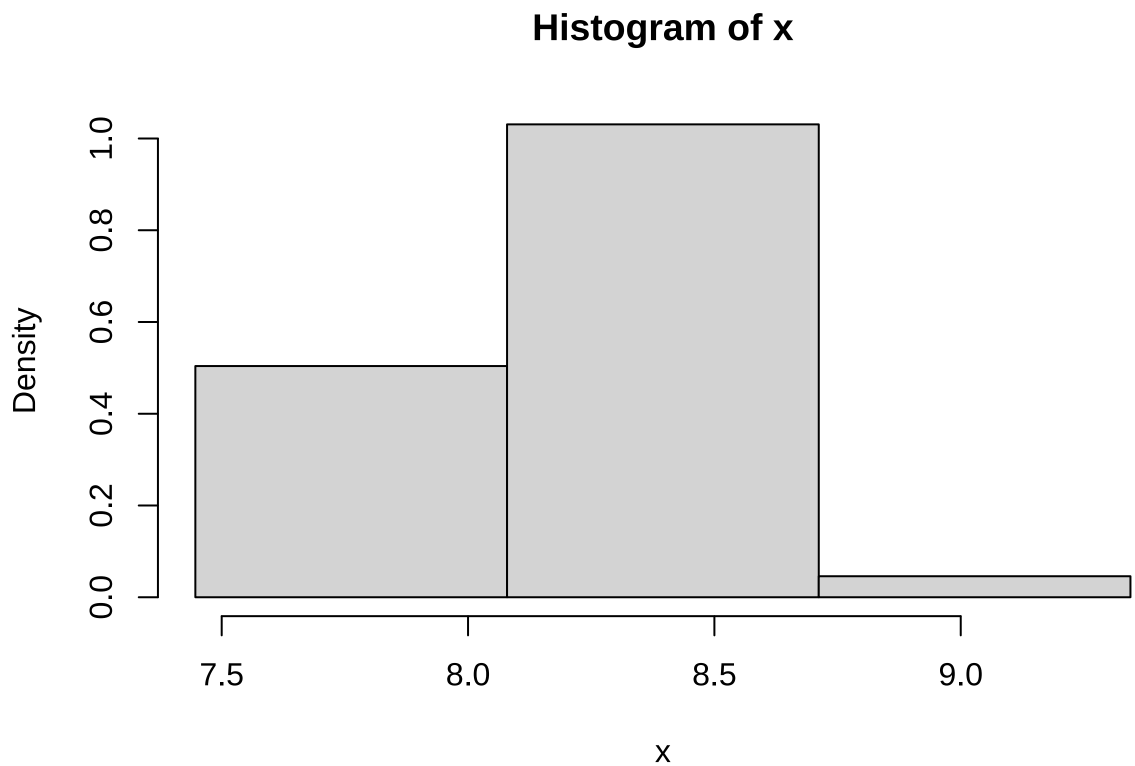

Histogram of x
Density
0.0
0.2
0.4
0.6
0.8
1.0
1.2
7.5
8.0
8.5
9.0
x


Histogram of x
Density
0.0
0.2
0.4
0.6
0.8
1.0
7.5
8.0
8.5
9.0
x

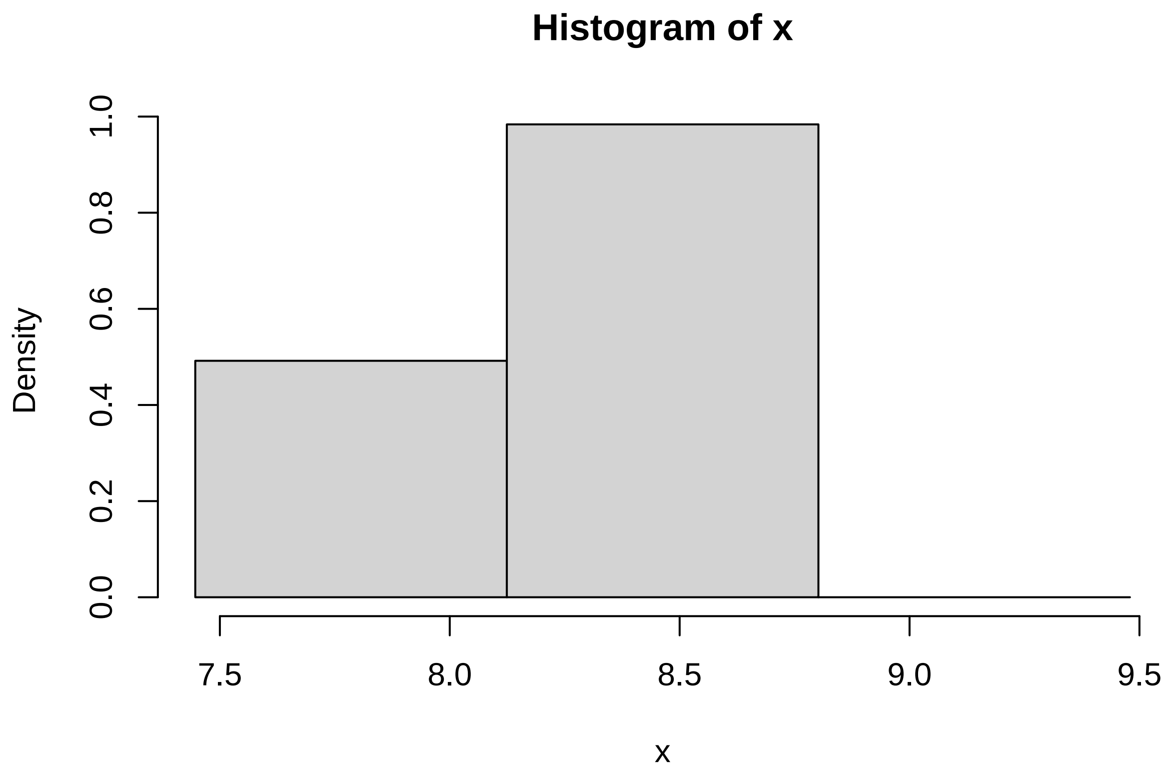

Histogram of x
Density
0.0
0.2
0.4
0.6
0.8
1.0
7.5
8.0
8.5
x

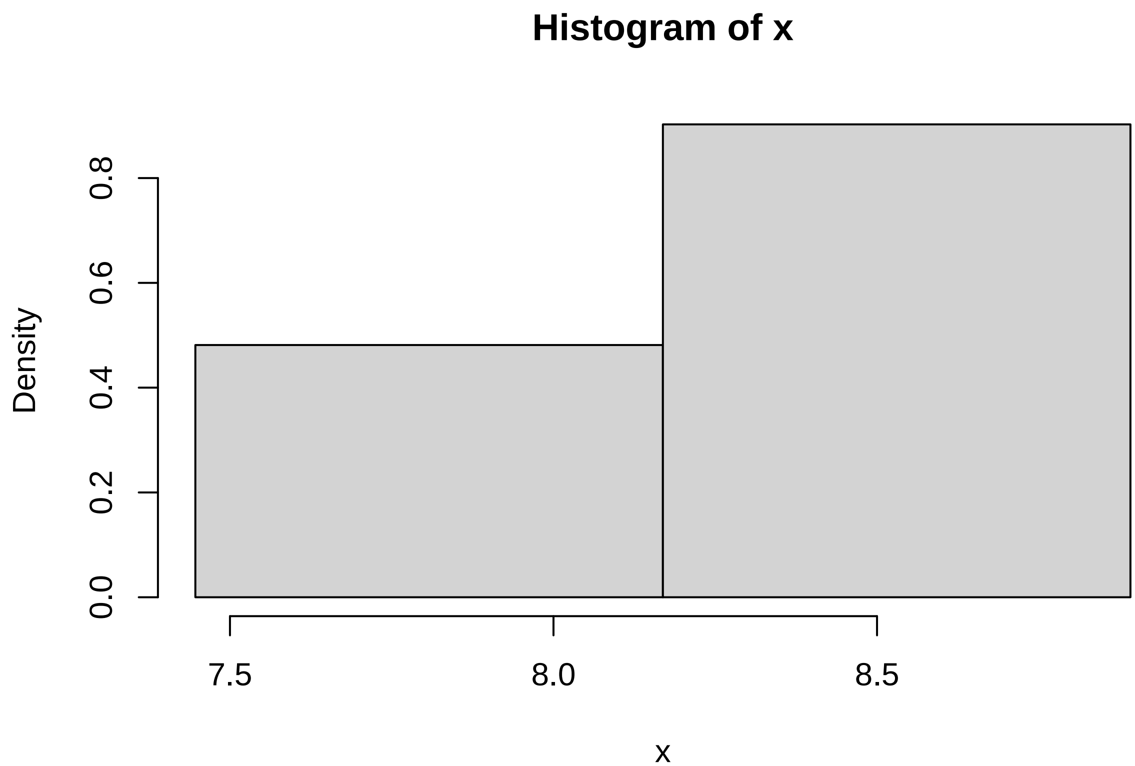

Histogram of x
Density
0.0
0.4
0.8
1.2
7.5
8.0
8.5
9.0
x

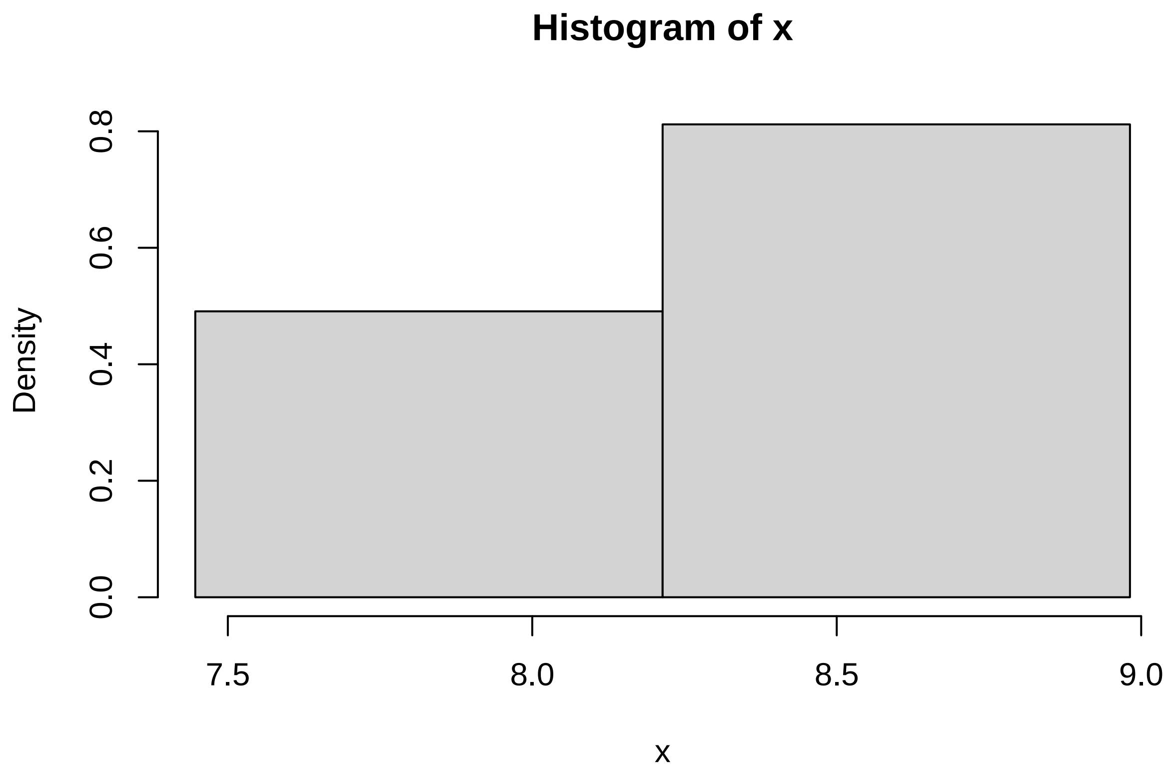

Histogram of x
Density
0.0
0.2
0.4
0.6
0.8
1.0
7.5
8.0
8.5
9.0
x

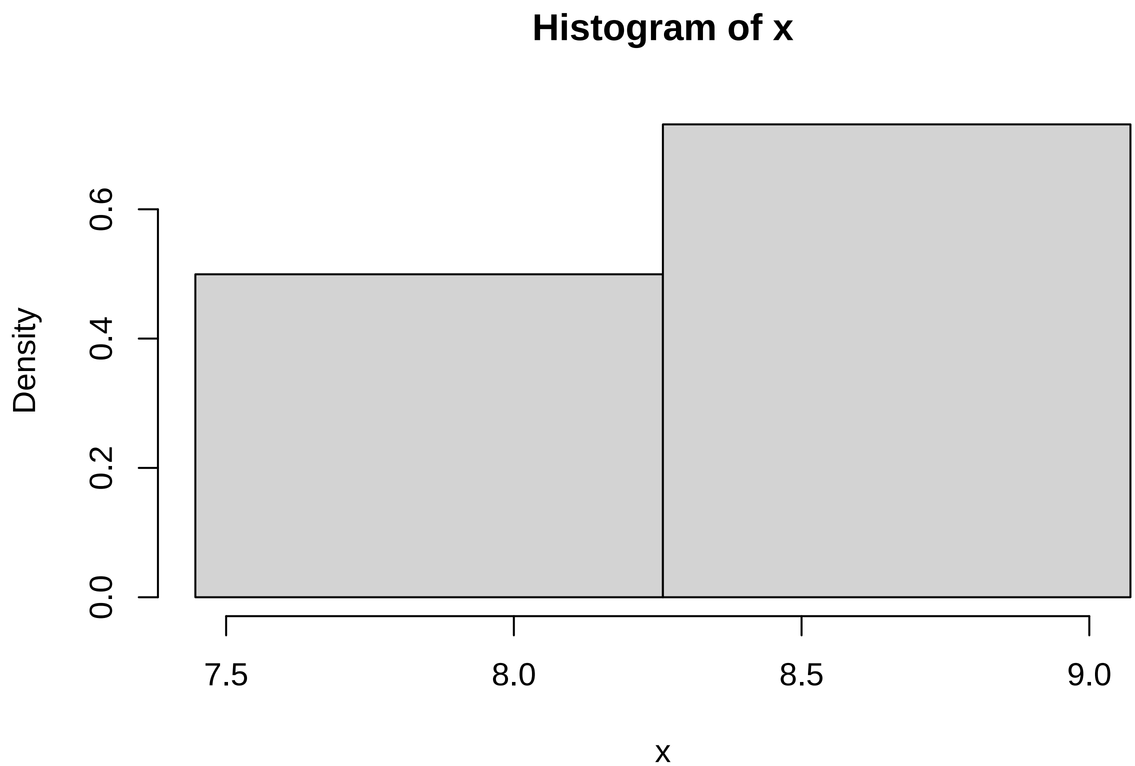


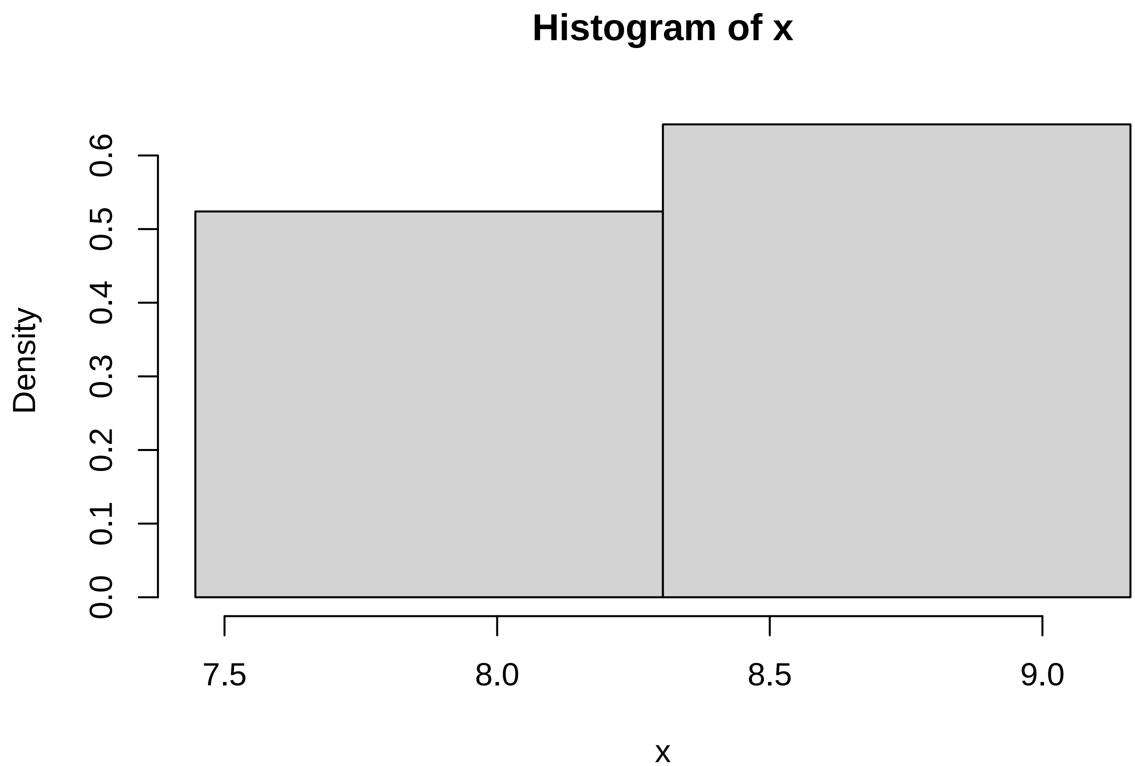
Histogram of x
Density
0.0
0.2
0.4
0.6
0.8
1.0
7.5
8.0
8.5
9.0
x

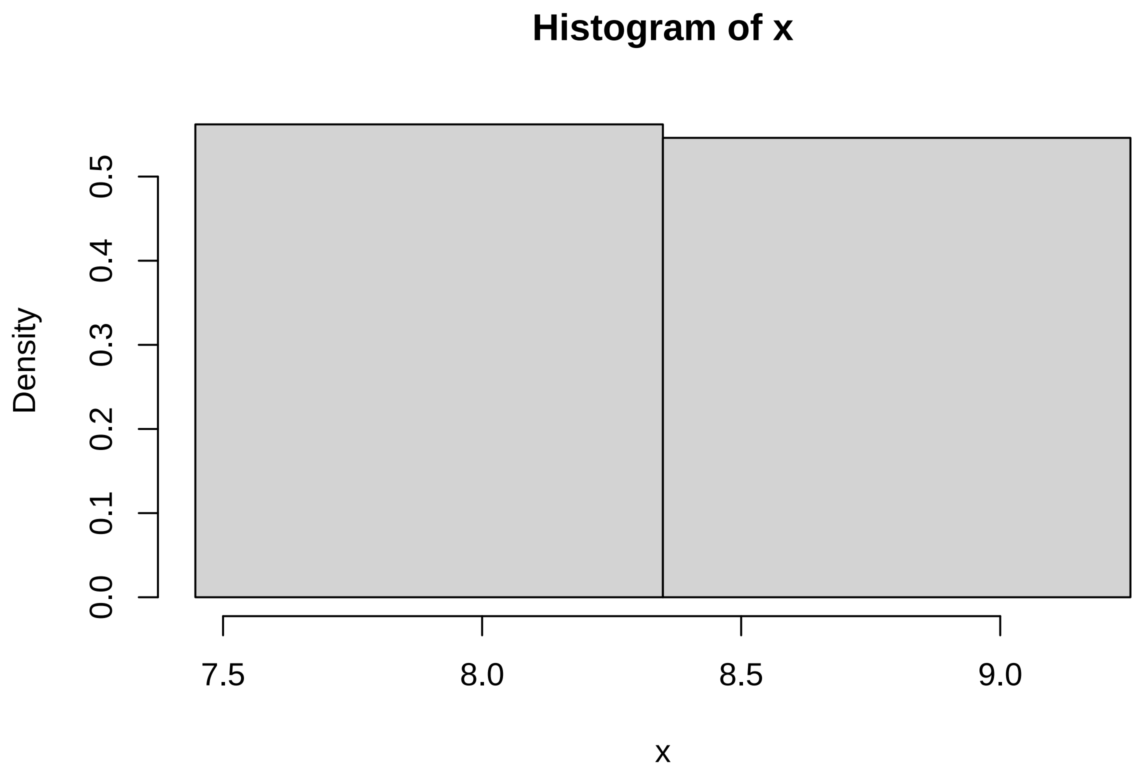

Histogram of x
Density
0.0
0.2
0.4
0.6
0.8
1.0
7.5
8.0
8.5
9.0
9.5
x

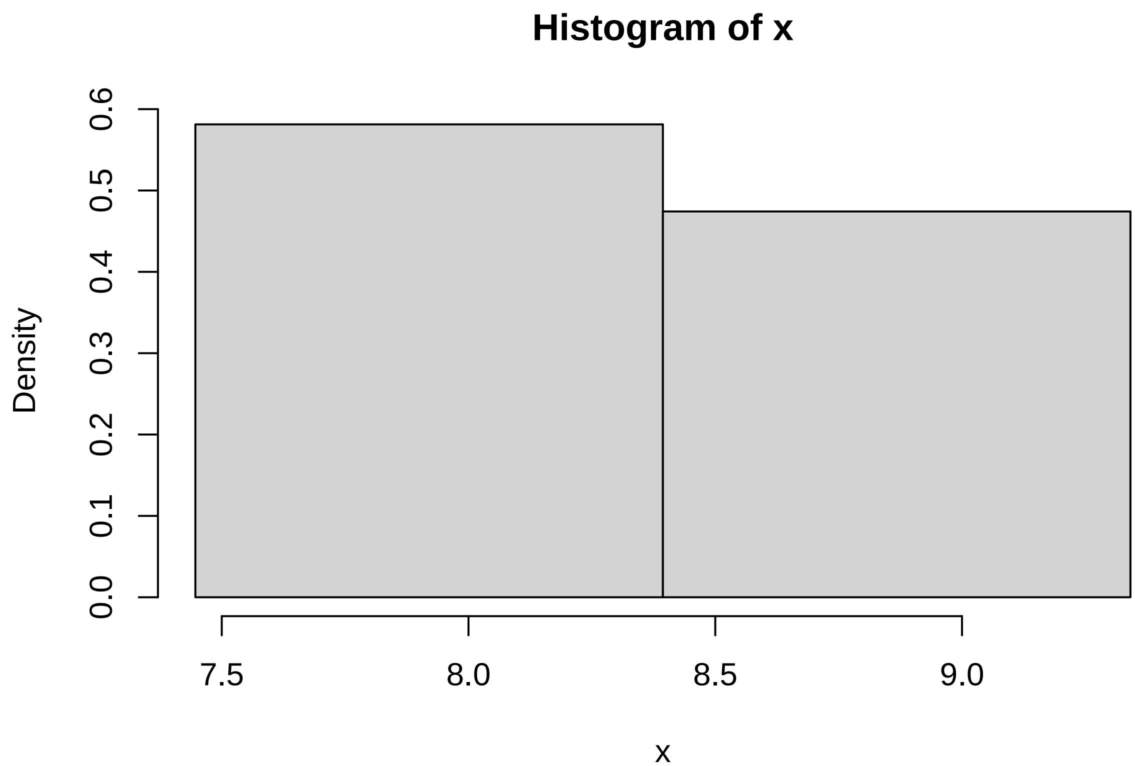

Histogram of x
Density
0.0
0.2
0.4
0.6
0.8
7.5
8.0
8.5
x

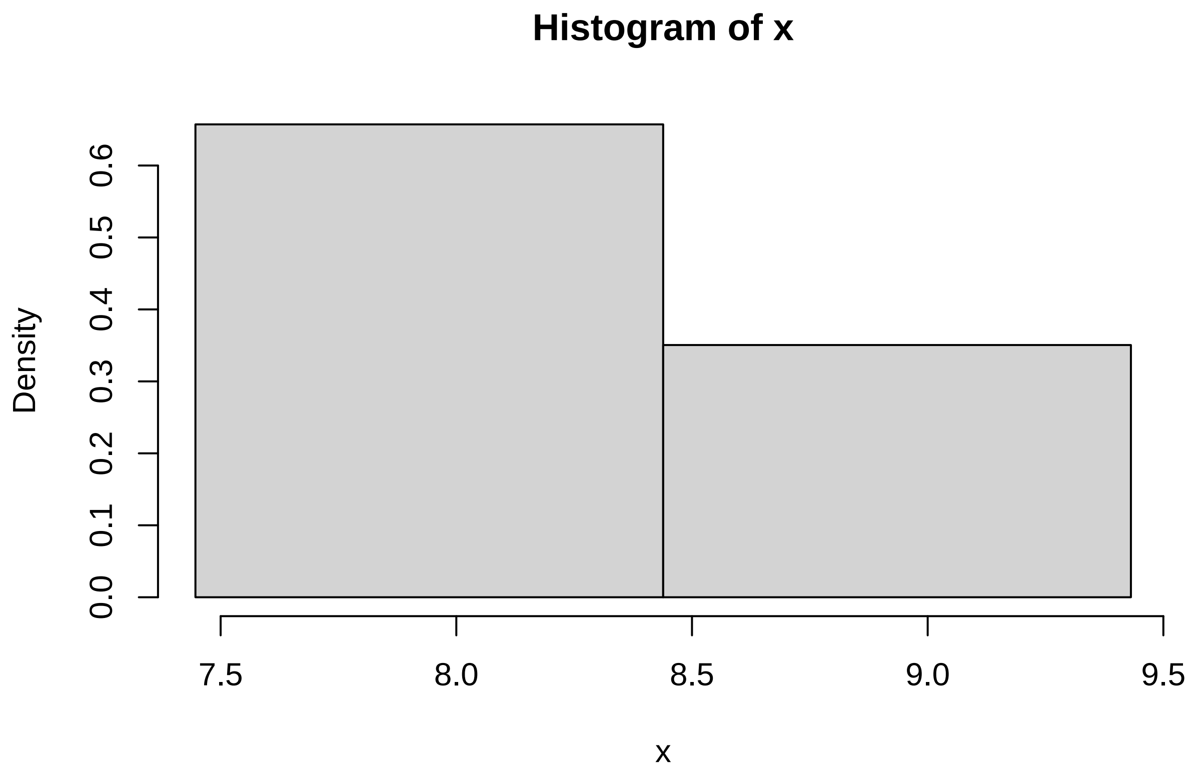

Histogram of x
Density
0.0
0.2
0.4
0.6
0.8
7.5
8.0
8.5
9.0
x

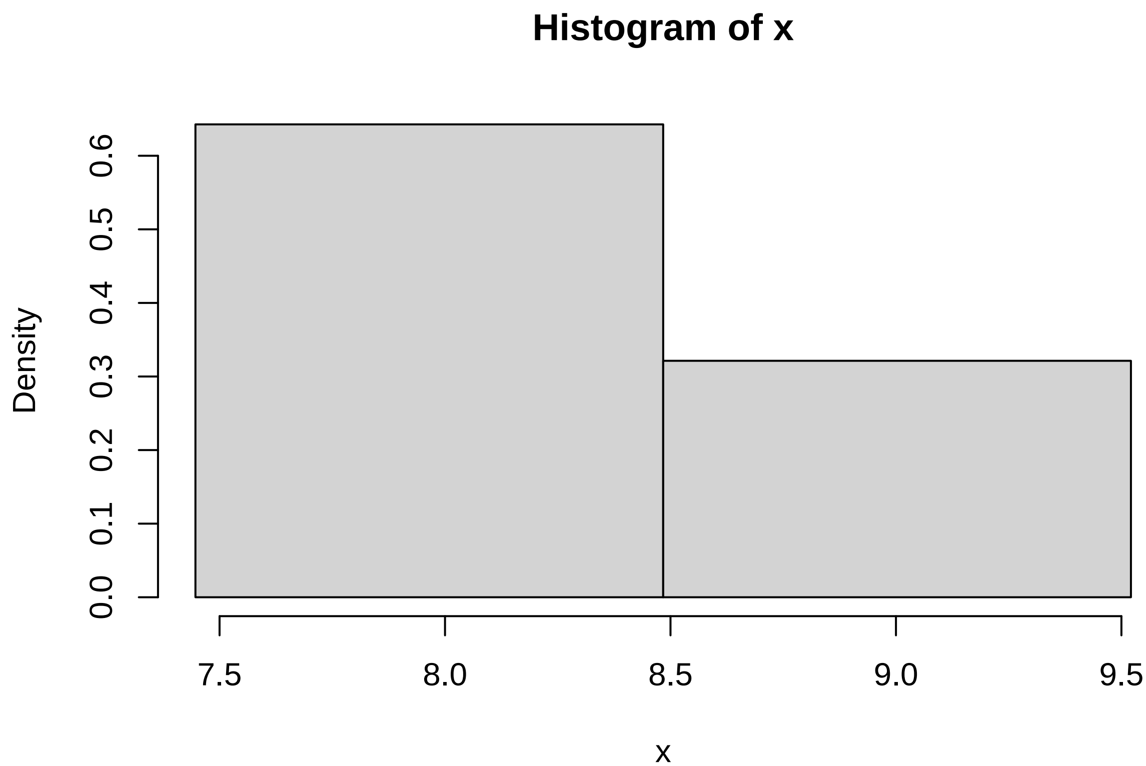

Histogram of x
Density
0.0
0.2
0.4
0.6
7.5
8.0
8.5
9.0
x

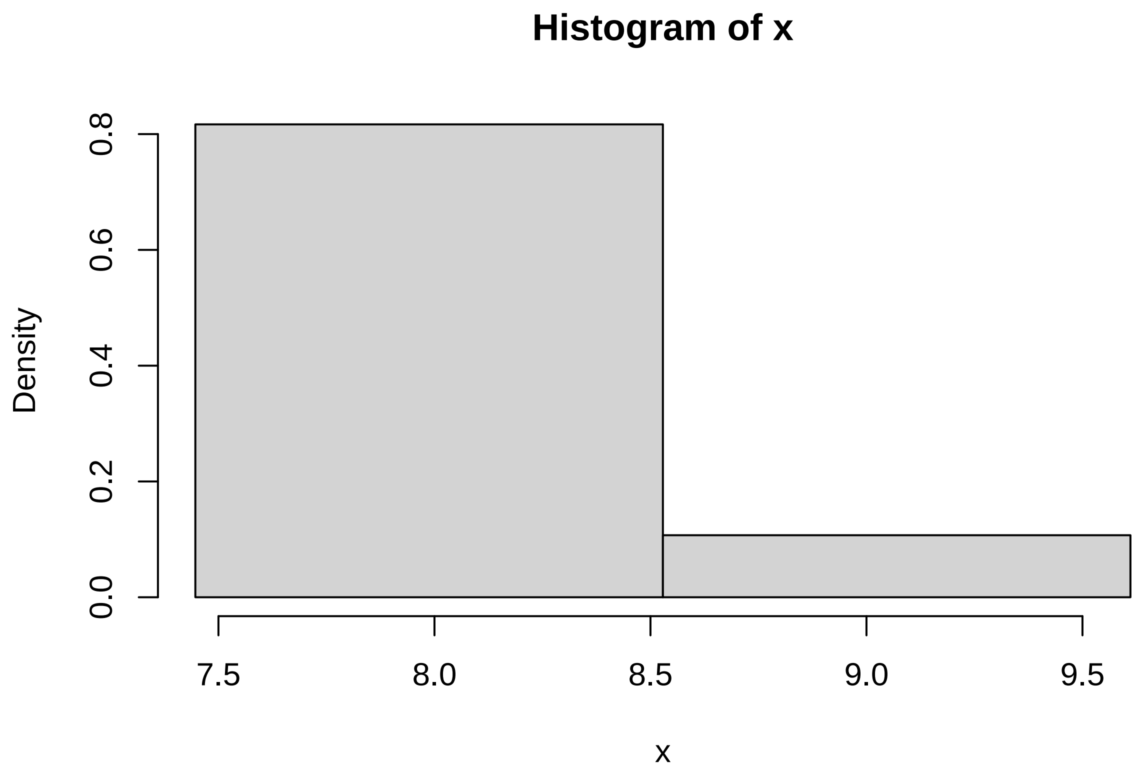

Histogram of x
Density
0.0
0.1
0.2
0.3
0.4
0.5
0.6
7.5
8.0
8.5
9.0
x

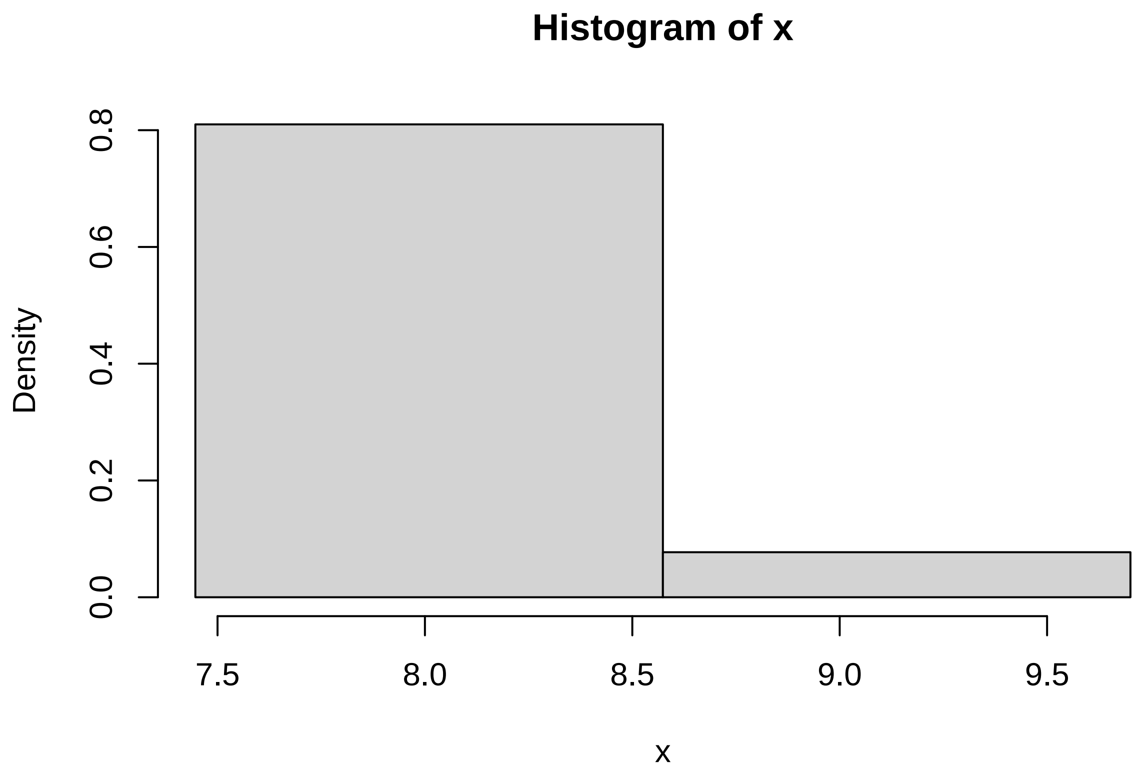

Histogram of x
Density
0.0
0.1
0.2
0.3
0.4
0.5
7.5
8.0
8.5
9.0
x


Histogram of x
Density
0.0
0.1
0.2
0.3
0.4
0.5
0.6
7.5
8.0
8.5
9.0
x

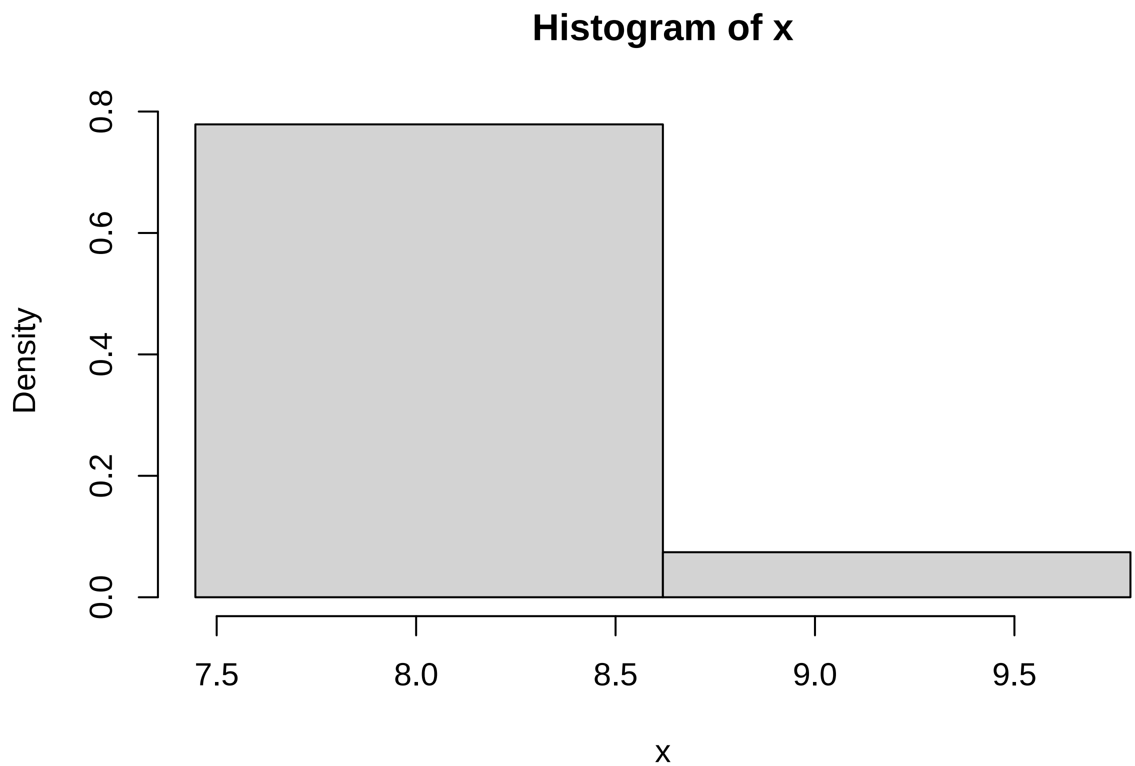

Histogram of x
Density
0.0
0.1
0.2
0.3
0.4
0.5
0.6
7.5
8.0
8.5
9.0
9.5
x

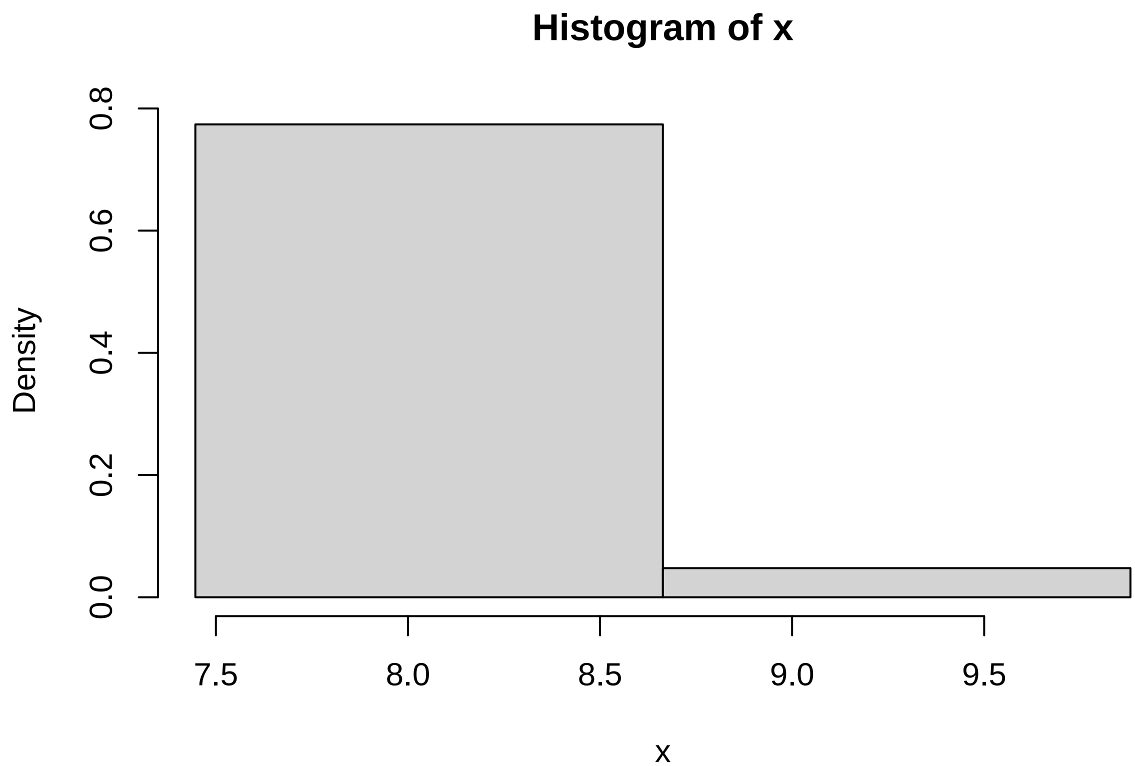

Histogram of x
Density
0.0
0.1
0.2
0.3
0.4
0.5
0.6
7.5
8.0
8.5
9.0
9.5
x

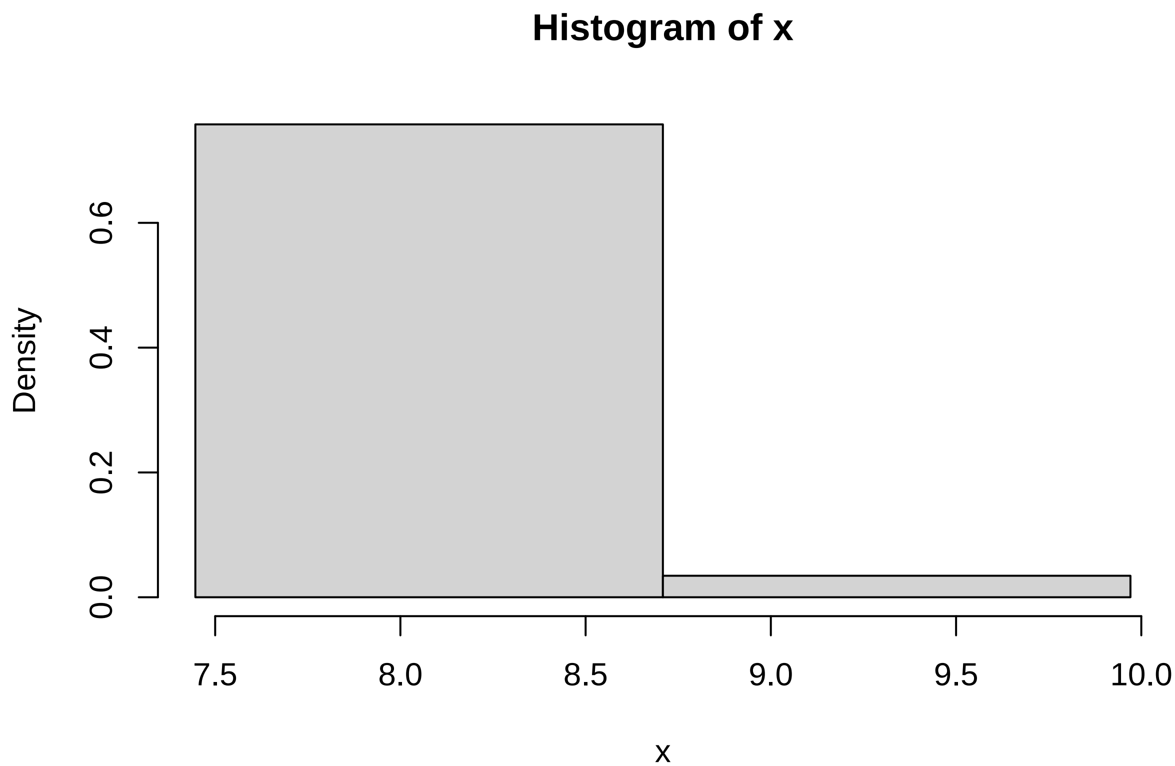

Histogram of x
Density
0.0
0.2
0.4
0.6
0.8
7.5
8.0
8.5
9.0
9.5
x

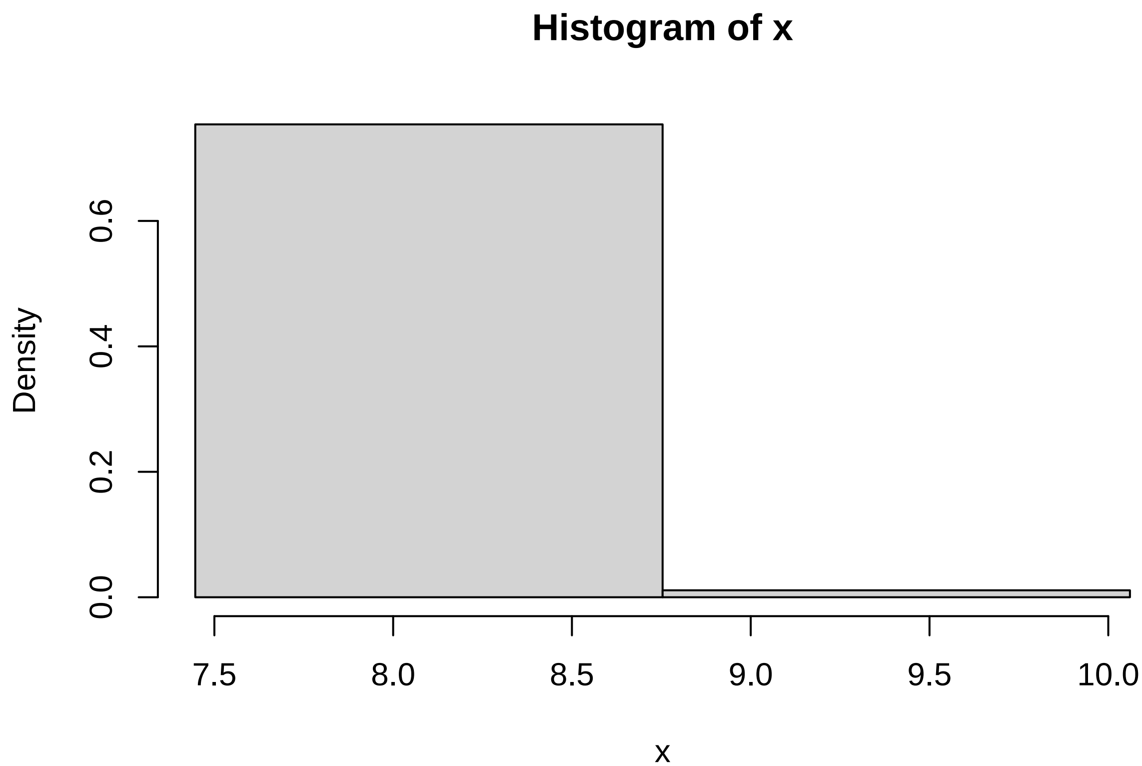


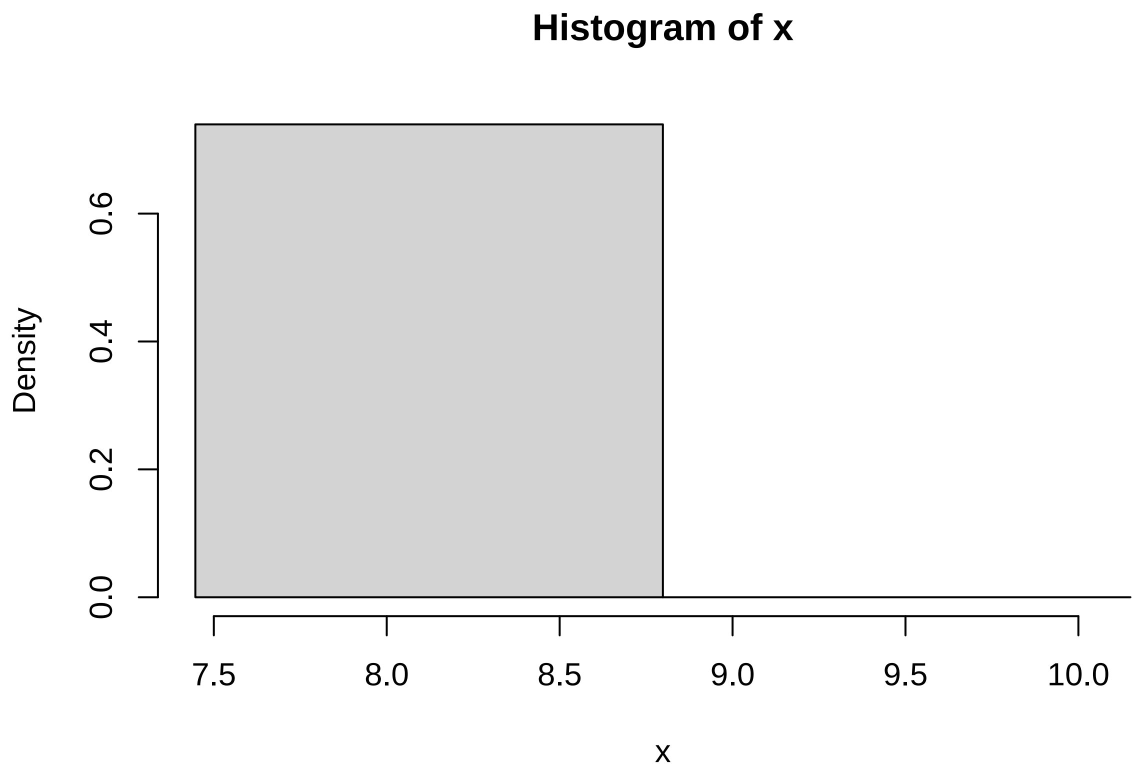
Histogram of x
Density
0.0
0.2
0.4
0.6
0.8
7.5
8.0
8.5
9.0
9.5
x

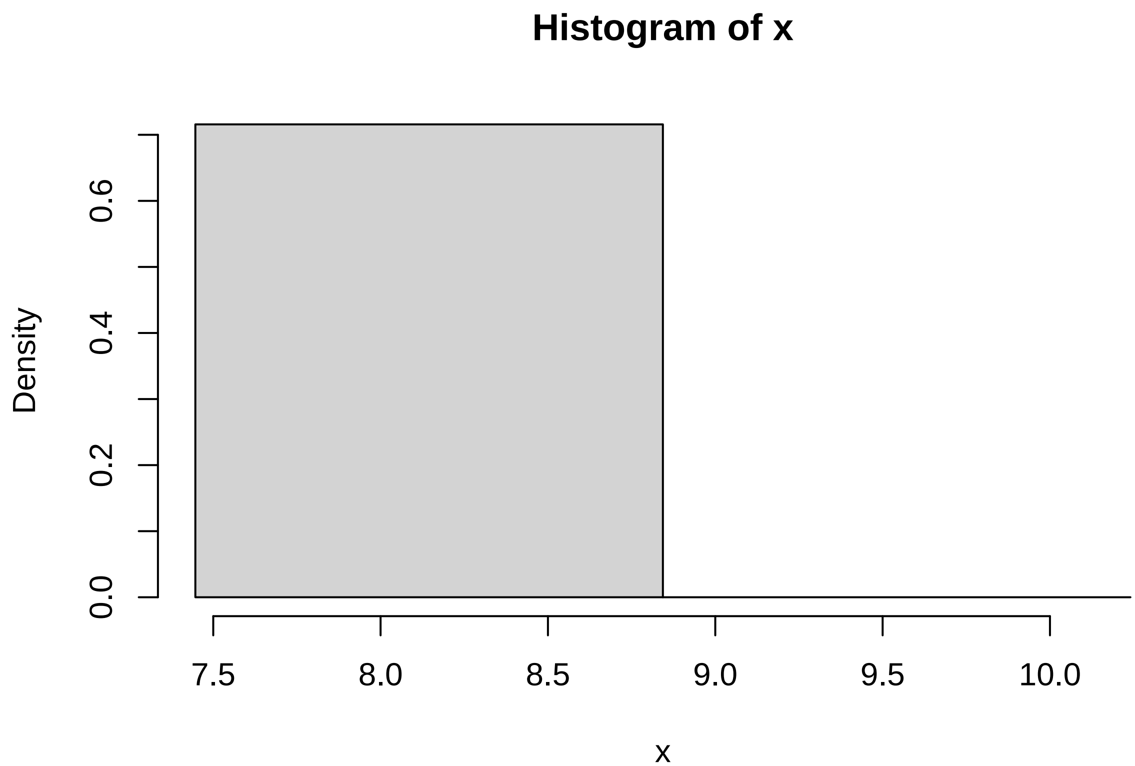

Histogram of x
Density
0.0
0.2
0.4
0.6
0.8
7.5
8.0
8.5
9.0
9.5
x


Histogram of x
Density
0.0
0.2
0.4
0.6
0.8
7.5
8.0
8.5
9.0
9.5
x


Histogram of x
Density
0.0
0.2
0.4
0.6
7.5
8.0
8.5
9.0
9.5
10.0
x


Histogram of x
Density
0.0
0.2
0.4
0.6
7.5
8.0
8.5
9.0
9.5
10.0
x


Histogram of x
Density
0.0
0.2
0.4
0.6
7.5
8.0
8.5
9.0
9.5
10.0
x



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:

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

.

```
# TODO
```

Kernel density estimator

8.

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