Stat 243 Final Project

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The approach we took to implement an adaptive rejection sampling algorithm, unsurprisingly, began with and mirrored the Gilks paper. The first task was to understand what our algorithm should do, and then begin to use R to implement a solution. To accomplish this required some manipulation of the given formulas to allows us to use the inverse CDF method in order to get the $x*$ values. Below are the calculations we used and then implemented in R:

First thing we need to do is to calculate the area under different *Upper* functions. Since *Upper* is a piece-wise function, we have to calculate the areas piece by piece. For the jth piece, we can calculate each piece by the following common expressions for *Upper* by using the equation for z_j below:

$$z_j = \frac{h(x_{j+1}) - h(x_j) - x_{j+1}h^{'}(x - j + 1) + x_j h^{'}(x_j)}{h^{'}(x_j) - h^{'}(x_{j+1})} \tag{1}$$

$$ExpUpper[j] = \int_{z_{j-1}}^{z_j} exp(h(x_j) + (x - x_j)h'(x_j)) \tag{2}$$

After some simple algebra, we can get the final expression as follows:

$$\frac{exp(h(x_j) - x_j h'(x_j))}{h'(x_j)} \cdot (exp(z_j h' x_j) - exp(z_{j-1}h'(x_j))) \tag{3}$$

We can find each piece of the area by changing different js. In our method, we use this expression to give us a vector that stores all the pieces and calculates a cumulative sum of this vector to stand for the cumulative area sums.

For the sampling process, we can use the inverse CDF method. But for this question, since the CDF is a piece wise function, we need to figure out which section the random number falls in. Then we should take the previous areas out of the overall CDF and use an inverse CDF method to draw samples in the section we are in.

More explicitly, the inverse CDF method first gets a uniform random number from 0 to 1 and then multiplies this number by the sum of the area, matching the total area. For simplicity, we call the $\int_{ub}^{lb} exp(u_k(x'))dx'$ as c, where c is a constant. Then we call the random number we generated as u as below:

$$uc - cum[j] = \int_{z_j}^{x} exp(h(x_j) + (x^* - x_j)h'(x_j))dx \tag{4}$$

We can easily calculate the $x*$ values as x_all:

$$x^* = \frac{1}{h'(x_j)} \cdot log(e^{(h'(x_j))} + (\frac{(uc - cum[j])h'(x_j)}{e^{h(x_j)} - x_j h'(x_j)})) \tag{5}$$

Once we had all the equations we needed, we began implementing them in R. In order to keep the code modular, each formula was created as a single function that we could call within the final ars algorithm. The functions we wrote based on the Gilks paper are *ConstructZ* function, *Envelope* function (S function from the paper), *Upper* function (U_k function from the paper), *ExpUpper* (exponential Upper function) and *Lower* function (l_k function from the paper). We chose to write the code modularly for a a few reasons: to increase the readability of the code, to decrease probability of bugs and to follow general best practices.

In order to handle the different inputs, and verify the ars function is used properly, we also added a few checks at the beginning of the function to check for the uniform and exponential density cases, since these can be more difficult to handle than other densities. First, we find the maximum of the log of the input density using the optimize function. We also find the mode of the function if the user does not provide initial x values (x_init) in order to initialize the starting values. After running these initial values through

the various smaller functions, we use GenCandidates to get some initial values of $x*$ to then pass to the RejectionTest function. This Rejection function will determine which $x*$ values to keep in the final sample and which to throw out based on the two inequalities in Gilks. Finally, we place the entire process into a while loop that ends when we hit the requisite number of $x*$ values in the returned samples.

To formally test our algorithm, we decided to use the Kolmogorov-Smirnov Test (KS Test) to measure the maximum difference between the empirical CDF we got from our algorithm and the theoretical CDF (a known truth). We set tolerances to be relatively low to ensure that passing was only possible if our algorithm worked correctly. Our formal tests include 7 continuous distributions that are easily called within R:

Normal
Gamma
Uniform
Beta
Chi-Square
Exponential
Weibull

Our tests also report the KS statistic for each distribution tested in order to see relative accuracy among them.

Our unit tests cover the *ConstructZ* function, *logconc* function, *findmax* function, *utest* function, and the *Upper* and *Lower* functions. In order to test these, we used known truths about the function output and tested them with the actual function output. If the two were essentially equal (with a low tolerance) then we can assume our functions work as intended. For example, to test the *utest* function, which detects whether the input density is uniform, we made sure the output was TRUE when the input was infact uniform and FALSE otherwise. Since the *GenCandidates* and *Rejection* functions are the main engines behind the *ars* algorithm, the formal tests essentially serve as their unit tests. It is also very difficult to come up with known truths about the output of these functions by themselves, and not in the context of the algorithm, which also contributed to our decision not to use the formal tests as their unit testing.

Finally, the individual team members contributed as follows:
Yuchao:
Auyon:
Qingyuan: Qingyuan contributed to the project with the discussion of the algorithm listed in the reference paper and debugging as the algorithm was implemented using R code. She also helped with the unit test and contributed to the write up of the final paper.
Alanna: Alanna contributed to the project with the discussion of the approach to the algorithm, code review as the algorithm was being constructed and bug fixes throughout. She also helped write some of the informal tests/checks within the algorithm (check for log concavity for example) as well as the unit tests. Finally, she contributed to the final project output by writing the the first draft of the algorithm overview as well as placing the ars function and its tests into an R package.

The github username that holds the final .tar.gz file is: amandazhang (https://github.com/amandazhang)

```
#### Adaptive Rejection Sampling ####
library(numDeriv)

## Take log of input function ##
h <- function(x){
  return(log(g(x)))
}

## Function that tests for log concavity ##
```

```
logconc <- function(h,lb,ub) {

  #log concave test here
  p <- runif(10000, min = 0, max = 1)

  #tests log concavity
  result <- h(p*lb + (1-p)*ub) >= p*h(lb) + (1-p)*h(ub)

  #result is 10000 TRUE's for the 10000 in p
  t <- rep(TRUE, 10000)
  finalreturn <- all.equal(t, result)

  #if returns TRUE then all elements are equal and 10000 reps were log concave so log concave
  if (finalreturn == FALSE) {
    stop("Density input to ars likely not log-concave. Please check and try again.")
  }
}

## Test for uniform case ##
utest <- function(g, lb, ub) {
  d <- (ub-lb)/100
  delta <- (ub - lb)/100
  x <- seq(lb + delta, ub - delta, by = d)
  dgvals <- grad(g, x)
  t <- rep(0,length(x))
  finalreturn <- all.equal(t, dgvals)
  if (finalreturn == TRUE) {
    uniformcase <- TRUE
  } else {
    uniformcase <- FALSE
  }
  return(uniformcase)
}

## Find optimum function and X_init ##
findmax <- function(h,lb,ub) {
  delta <- (ub - lb)/1000
  max <- optimize(f = h, interval = c(lb, ub), lower = lb, upper = ub, maximum = TRUE)$maximum
  #taking care of exp case
  if (abs(max - ub) < .0001) {
    rp <- max
    mid <- max - .5*delta
    lp <- (max - delta)
    X_init <- c(lp,mid,rp)
  } else if (abs(max - lb) < .0001) {
    rp <- (max + delta)
    mid <- max + .5*delta
    lp <- max
    X_init <- c(lp,rp)
  } else {
    rp <- (max + delta)
    lp <- (max - delta)
    X_init <- c(lp,max,rp)
```

```
  }
  return(X_init)
}

## Compute intersection points of tangents, z ##
ConstructZ <- function(x,h,lb,ub){
  k = length(x)
  x_j1 <- c(0,x)
  x_j <- c(x,0)
  Num <- h(x_j1)-h(x_j)-x_j1*grad(h,x_j1)+x_j*grad(h,x_j)
  Den <- grad(h,x_j)-grad(h,x_j1)

  if(sum(abs(Den),na.rm = TRUE)<1e-6){

    tmp <-  (x[-1] + x[-k])/2
    tmp <- c(lb+1e-4,tmp,ub)

  }else{

    tmp <- Num/Den
    tmp[1] <- lb
    tmp[length(x)+1] <- ub
  }
  return(tmp)
}

## Lower bound, l(x) ##
Lower <- function(x,H_k,dH_k,X_k){

  if(x < min(X_k) | x > max(X_k)){
    return(-Inf)
  }else{
    j <- max(which(x >= X_k))
    Num <- (X_k[j+1]-x)*H_k[j] + (x-X_k[j])*H_k[j+1]
    Den <- X_k[j+1] - X_k[j]
    return(Num/Den)
  }
}

## Upper bound, u(x) ##
Upper <- function(x,H_k,dH_k,X_k,Z_k){
  j <- min(which(x < Z_k)-1)
  return(H_k[j] + (x - X_k[j]) * dH_k[j])
}

## Exponentiated upper bound, exp(u(x)) ##
ExpUpper <- function(x,H_k,dH_k,X_k,Z_k){
  return(exp(Upper(x,H_k,dH_k,X_k,Z_k)))
}

## Normalized version of exponentiated upper bound, s(x) ##
Envelope <- function(x,C,H_k,dH_k,X_k,Z_k){
```

```
  return(ExpUpper(x,H_k,dH_k,X_k,Z_k)/C)
}

## Generate candidate samples by sampling from envelope s(x) ##
# We sample from the inverse CDF of the envelope by first randomly selection a segment of the envelope,
# the selected segment as a PDF supported by the adjacent Z_k points
GenCandidates <- function(u,cum_area_env,H_k,X_k,dH_k,Z_k,areas_u){
  j <- max(which(u > cum_area_env))
  if(dH_k[j] == 0){
    x <- runif(1, Z_k[j],Z_k[j+1])
    return(x)
  }else{

    # Sample from uniform random
    w = runif(1)

    # Scale seed value w to area of the selected segment, since area under segment is not equal to 1
    w_sc = w*(1/areas_u[j])*exp(H_k[j] - X_k[j]*dH_k[j])*(exp(dH_k[j]*Z_k[j+1]) -exp(dH_k[j]*Z_k[j]))

    # Use inverse CDF of selected segment to generate a sample
    x = (1/dH_k[j])*log(w_sc*areas_u[j]/(exp(H_k[j] - X_k[j]*dH_k[j])) + exp(Z_k[j]*dH_k[j]))
  }
  return(x)
}

## Apply squeeze and rejection test to each candidate sample ##
RejectionTest <- function(x,H_k,dH_k,X_k,Z_k){

  # Generate random seed
  w = runif(1)

  # Initialize squeeze and reject tests, and indicator for adding point
  squeeze = FALSE
  accept = FALSE
  add = FALSE

  # Compute threshold values for failing squeeze and rejection tests
  l_threshold = exp(Lower(x,H_k,dH_k,X_k) - Upper(x,H_k,dH_k,X_k,Z_k))
  u_threshold = exp(h(x) - Upper(x,H_k,dH_k,X_k,Z_k))

  #print(l_threshold)
  if( w <= l_threshold){

    squeeze = TRUE
    accept = TRUE

  }else if(w <= u_threshold){

    squeeze = FALSE
    accept = TRUE

  }else{
```

```
    accept = FALSE
  }

  # Determine whether to add point to abscissae
  if(squeeze*accept==FALSE) add = TRUE

  # Return boolean indicating whether to accept candidate sample point
  return(list(rej=squeeze+accept,add=add))
}

#' Adaptive Rejection Sampling (ars) Function
#'
#' Adaptive rejection sampling function that creates a sample
#' from a density function based on the Gilks(1992) paper.
#'
#' @param g probability density function, as a function of x (e.g. g <- function(x) dnorm(x,1,2))
#' @param n number of values the final sample should contain
#' @param lb lower bound to evaluate the density on
#' @param ub upper bound to evaluate the density on
#' @param X_init optional vector of initial values, default = NULL
#' @param batchsize optional argument to adjust number of x* values to evaluate at once
#' @return sample of with specified (n) elements
#' @export

################################################################################

### Main ARS function ###
ars <- function(g,n,lb,ub,X_init = NULL, batchsize = round(n/100)){

  # Test for uniform case
  uniftest <- utest(g, lb, ub)

  if(uniftest == TRUE) {
    x_all <- runif(n,lb,ub)
    return(x_all)
  }
  # Compute log of input function
  h <- function(x){
    return(log(g(x)))
  }

  if (is.null(X_init) == TRUE) {
    X_k <- findmax(h,lb,ub)
  } else {
    X_k <- X_init
  }

  # Initialize abscissae and sample points
  x_all = NULL

  while(length(x_all)<n){

    # Compute intersection points
```

```
    Z_k <- ConstructZ(X_k,h,lb,ub)

    # Store h and h' values
    H_k <- h(X_k)
    dH_k <- grad(h, X_k)

    # Calculate areas under exponential upper bound function for normalization purposes
    areas_u = unlist(sapply(2:length(Z_k),function(i){integrate(ExpUpper,Z_k[i-1],Z_k[i],H_k,dH_k,X_k,Z_
    C = sum(areas_u)

    # compute cumulative areas under envelope, which will sum to 1
    areas_env = areas_u/C
    cum_area_env <- cumsum(areas_env)
    cum_area_env <- c(0,cum_area_env)

    # Generate seeds for Inverse CDF method
    seeds <-runif(batchsize)

    # Generate candidate samples
    x_candidates <- sapply(seeds, GenCandidates, cum_area_env = cum_area_env, H_k = H_k, X_k = X_k,dH_k

    # Apply squeeze and rejection tests
    test_flag <- sapply(x_candidates,RejectionTest, H_k = H_k, X_k = X_k, dH_k = dH_k,Z_k = Z_k)
    keep_sample_flag <- test_flag[1,]
    add_X_k_flag <- test_flag[2,]

    # Filter out rejected points and update full set of samples
    x_keep <- x_candidates[keep_sample_flag>0]
    x_all = c(x_keep,x_all)

    # Identify samples to add to X_k
    X_new_k = x_candidates[add_X_k_flag>0]
    X_k = sort(c(X_k,X_new_k))
  }
  return(x_all)
}
```

This would declare all the functions I need in the environment.

```
#test for upper
  g<- dnorm
  X_k <- c(-1,0,1)
  lb <- -1
  ub <- 1
  H_k <- h(X_k)
  dH_k <- grad(h,X_k)
  Z_k <- ConstructZ(X_k, h, lb, ub)

  x <- seq(lb+0.01, ub-0.01, by = 0.01)
  y <- sapply(x, Upper, H_k = H_k, dH_k = dH_k, X_k = X_k, Z_k = Z_k)
  y
```

```
##   [1] -1.4089385 -1.3989385 -1.3889385 -1.3789385 -1.3689385 -1.3589385
##   [7] -1.3489385 -1.3389385 -1.3289385 -1.3189385 -1.3089385 -1.2989385
```

```
##  [13] -1.2889385 -1.2789385 -1.2689385 -1.2589385 -1.2489385 -1.2389385
##  [19] -1.2289385 -1.2189385 -1.2089385 -1.1989385 -1.1889385 -1.1789385
##  [25] -1.1689385 -1.1589385 -1.1489385 -1.1389385 -1.1289385 -1.1189385
##  [31] -1.1089385 -1.0989385 -1.0889385 -1.0789385 -1.0689385 -1.0589385
##  [37] -1.0489385 -1.0389385 -1.0289385 -1.0189385 -1.0089385 -0.9989385
##  [43] -0.9889385 -0.9789385 -0.9689385 -0.9589385 -0.9489385 -0.9389385
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## [127] -0.9189385 -0.9189385 -0.9189385 -0.9189385 -0.9189385 -0.9189385
## [133] -0.9189385 -0.9189385 -0.9189385 -0.9189385 -0.9189385 -0.9189385
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## [169] -1.1089385 -1.1189385 -1.1289385 -1.1389385 -1.1489385 -1.1589385
## [175] -1.1689385 -1.1789385 -1.1889385 -1.1989385 -1.2089385 -1.2189385
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## [187] -1.2889385 -1.2989385 -1.3089385 -1.3189385 -1.3289385 -1.3389385
## [193] -1.3489385 -1.3589385 -1.3689385 -1.3789385 -1.3889385 -1.3989385
## [199] -1.4089385
```
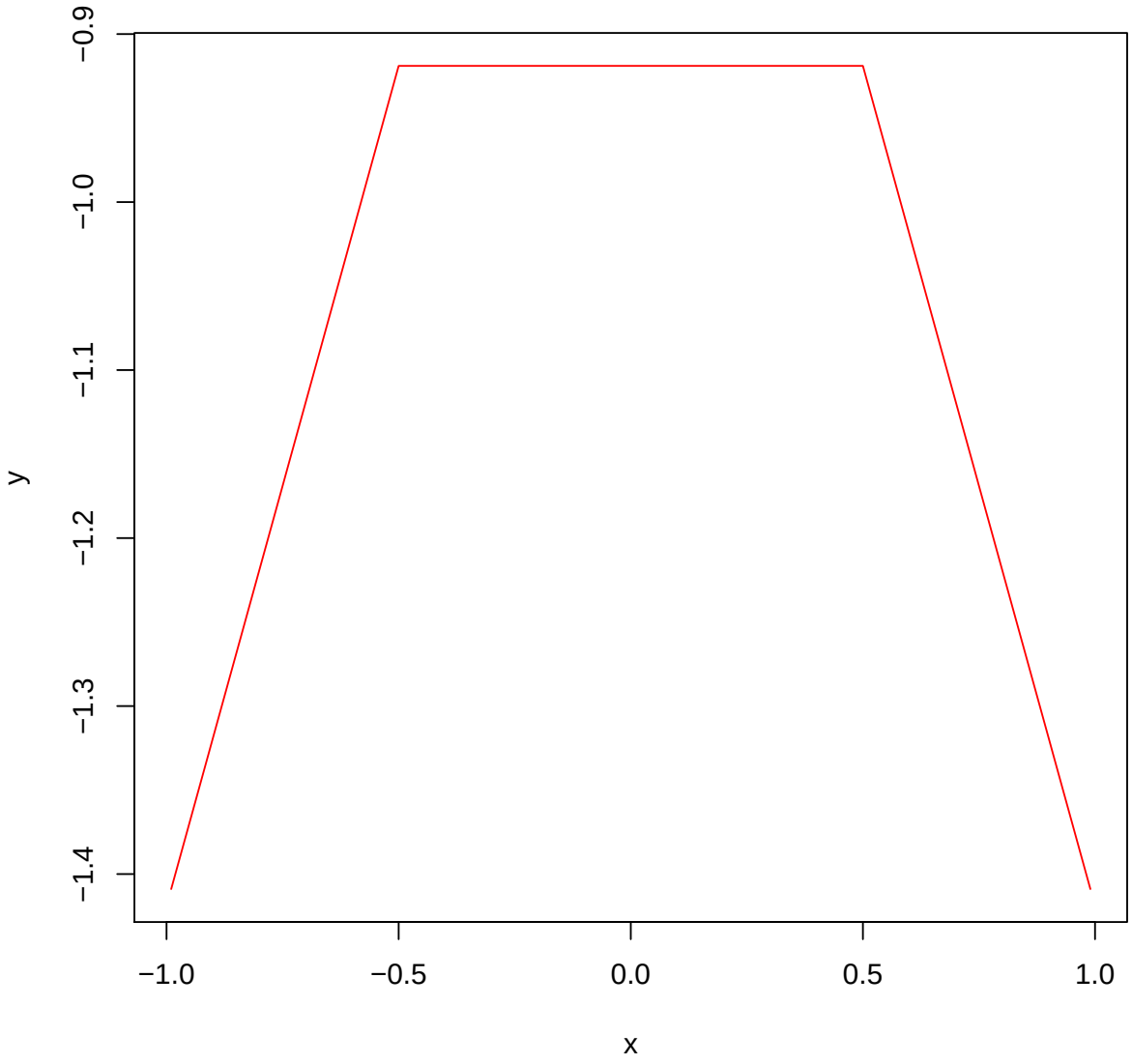

```
  plot(x,y, type = "l", col = "Red")
```



We will show the theoretic value matches the value we got.

```
#test for lower
  x_2 <- seq(lb+0.01, ub-0.01, by = 0.01)
  y_2 <- sapply(x_2, Lower, H_k = H_k, dH_k = dH_k, X_k = X_k)
  y_2
```

```
##   [1] -1.4139385 -1.4089385 -1.4039385 -1.3989385 -1.3939385 -1.3889385
##   [7] -1.3839385 -1.3789385 -1.3739385 -1.3689385 -1.3639385 -1.3589385
##  [13] -1.3539385 -1.3489385 -1.3439385 -1.3389385 -1.3339385 -1.3289385
##  [19] -1.3239385 -1.3189385 -1.3139385 -1.3089385 -1.3039385 -1.2989385
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##  [31] -1.2639385 -1.2589385 -1.2539385 -1.2489385 -1.2439385 -1.2389385
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##  [43] -1.2039385 -1.1989385 -1.1939385 -1.1889385 -1.1839385 -1.1789385
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##  [49] -1.1739385 -1.1689385 -1.1639385 -1.1589385 -1.1539385 -1.1489385
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## [163] -1.2339385 -1.2389385 -1.2439385 -1.2489385 -1.2539385 -1.2589385
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## [187] -1.3539385 -1.3589385 -1.3639385 -1.3689385 -1.3739385 -1.3789385
## [193] -1.3839385 -1.3889385 -1.3939385 -1.3989385 -1.4039385 -1.4089385
## [199] -1.4139385
```
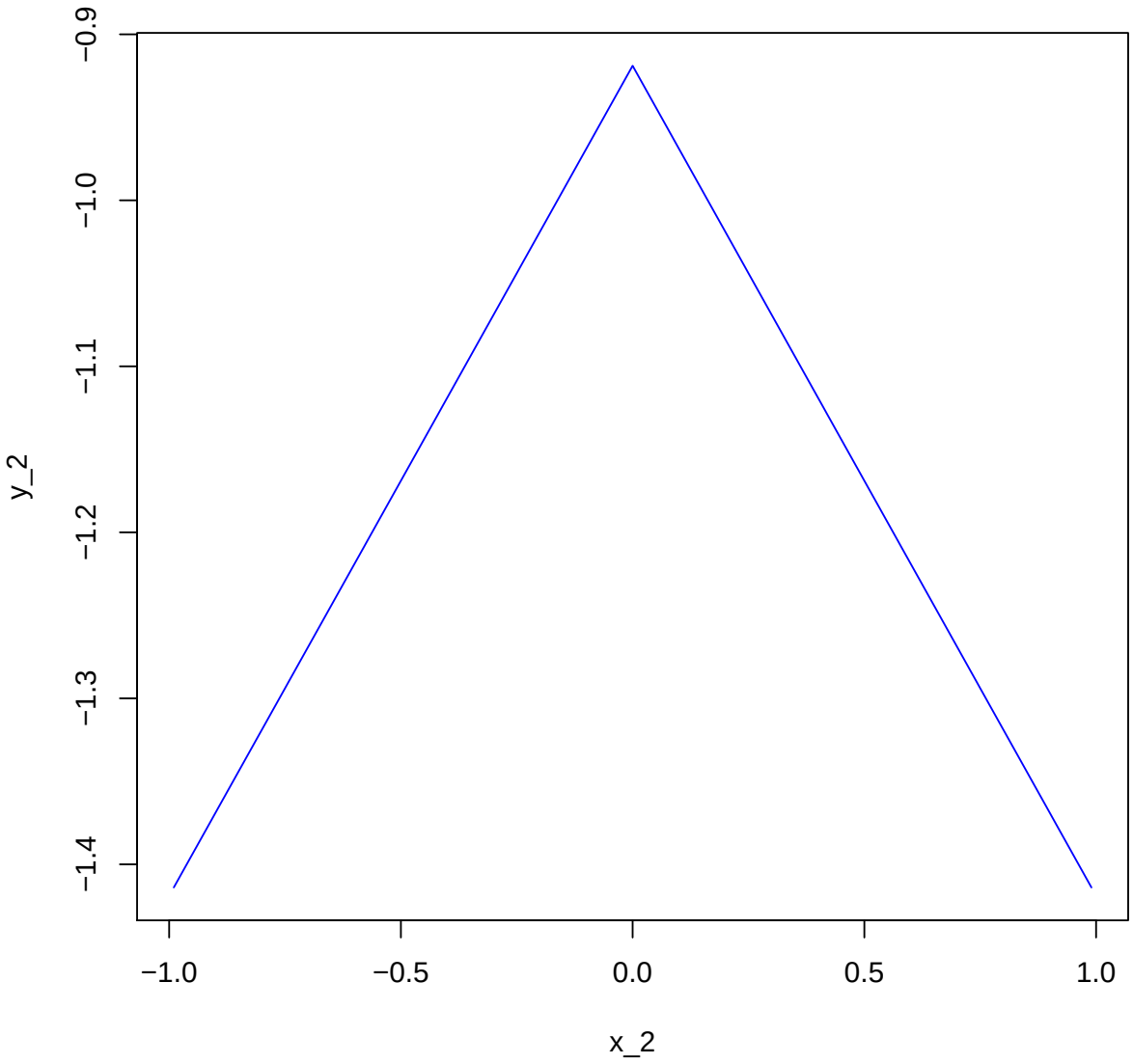
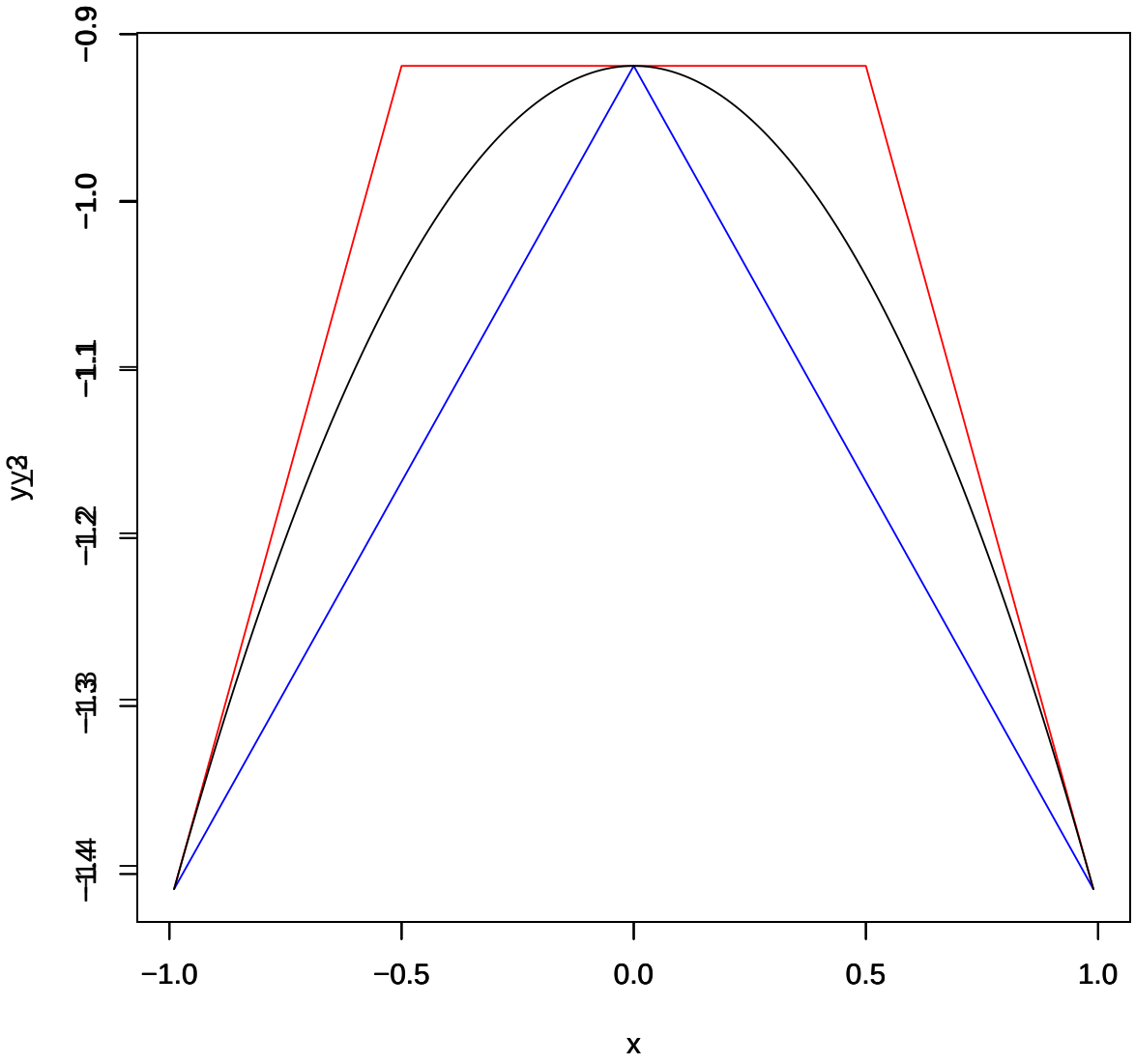

```
  plot(x_2,y_2, type = "l", col = "Blue")
```



We will show the theoretic value matches the value we got.

```
y_3 <- h(x)
plot(x,y, type = "l", col = "Red")
par(new = T)
plot(x,y_2, type = "l", col = "Blue")
par(new = T)
plot(x,y_3, type = "l", col = "Black")
```


−0.9
−1.0
−1.1
−1.2
−1.3
−1.4
yy2
−1.0
−0.5
0.0
0.5
1.0
x