

HUDM6026 Homework_05

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Q1:

Determine the first derivative of f and encode it in a function called `f_prime`.

MY SOLUTION:

Based on chain rule, the first derivative of $f(x)$ is

$$f(x)' = \frac{-2x}{x^2 + 1} + \frac{1}{3}x^{-\frac{2}{3}}$$

. Based on this equation, I write the code below. Certainly, we can use the R-built-in function to get the derivative quickly.

```
> f_prime <- function(x) {  
+   out_ <- (-2*x)/(x^2 + 1) + (1/3)*(x^(-2/3))  
+   return(out_)  
+ }  
> # since this question requires the maximum, I use -1 times the function.  
> f_prime_neg <- function(x){  
+   out_ <- (-2*x)/(x^2 + 1) + (1/3)*(x^(-2/3))  
+   out_ <- out_*(-1)  
+   return(out_)  
+ }
```

Q2:

Create a plot of f and f' on $[0,4]$ in different colors and line types and add a legend.

MY SOLUTION:

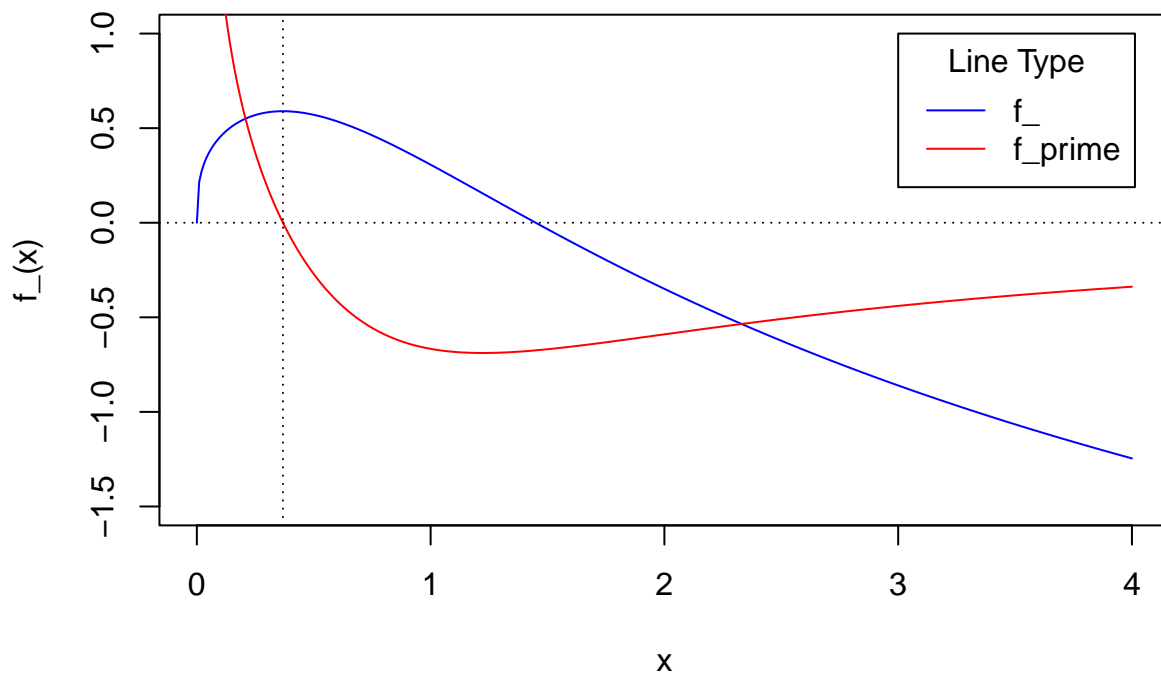
```
> # write the original function with the name of f_  
> f_ <- function(x){  
+   out_ <- (-1)*log(x^2 + 1) + x^(1/3)  
+   return(out_)  
+ }  
> # since this question requires the maximum, I use -1 times the function.  
> f_neg <- function(x){  
+   out_ <- (-1)*log(x^2 + 1) + x^(1/3)  
+   return(out_*(-1))  
+ }  
>  
> # first plot the original function  
> x <- seq(0,4,0.01)  
> # plot the original function with blue line  
> plot(x, f_(x), col="blue", type = "l", ylim = c(-1.5,1))
```

```

> # plot the first derivative with red line
> lines(x, f_prime(x), col="red", type = "l")
> # add the legend
> legend(3,1, inset = 0.1, c("f_", "f_prime"), lty = 1,
+       col = c("blue", "red"), title="Line Type")
> # add a horizontal line to indicate the y=0
> abline(h=0, lty=3)
> abline(v=0.3683525, lty=3)
> mtext("Figure 1. The Lines of the Given Function and it's First Derivative",
+       side = 3,
+       line = -2,
+       outer = T)

```

Figure 1. The Lines of the Given Function and it's First Derivative



Q3:

Finish the functions that I started in the R code notes for univariate optimization for the golden section search, the bisection method, and Newton's method.

MY SOLUTION:

3.1 The Golden Section Search

```

> golden <- function(f, int, precision = 1e-6)
+ {
+   rho <- (3-sqrt(5))/2 # ::: Golden ratio
+   # ::: Work out first iteration here
+   f_a <- f(int[1] + rho*(diff(int)))
+   f_b <- f(int[2] - rho*(diff(int)))
+   ### How many iterations will we need to reach the desired precision?
+   N <- ceiling(log(precision/(diff(int)))/log(1-rho))
+   for (i in 1:(N)) # index the number of iterations
+   {
+     if (f_a < f_b)
+     {
+       int[2] <- int[2] - rho*(diff(int))
+       f_b <- f(int[2])
+     } else{
+       if (f_a >= f_b)
+       {
+         int[1] <- int[1] + rho*(diff(int))
+         f_a <- f(int[1])
+       } }
+   }
+   int
+   print(paste0("Iteration for ",N," times;",
+               " The maximum value is at", round(int[1],6)))
+ }

```

3.2 The Bisection Method

More information about this method can be found on *Page 116* of Chong and Zak (2013).

```

> bisection <- function(f_prime, int, precision = 1e-7)
+ {
+   # ::: f_prime is the function for the first derivative
+   # ::: of f, int is an interval such as c(0,1) which
+   # ::: denotes the domain
+
+   N <- ceiling(log(precision/(diff(int)))/log(.5))
+   # find the midpoint of the initial uncertainty range
+   midpoint <- (int[1]+int[2]) /2
+   # evaluate the f_prime on the midpoint
+   f_prime_a <- f_prime(midpoint)
+   i <- 1
+   for (i in 1:N)
+   {
+     i <- i + 1
+     if(f_prime_a < 0)
+     {
+       # if the f_prime on the midpoint is less than 0,
+       # the minimizer must be on the right side of midpoint.
+       int[1] <- midpoint
+       # update the uncertainty range
+       midpoint <- (int[1]+int[2]) /2
+     }
+   }
+ }

```

```

+   } else
+     if(f_prime_a > 0)
+     {
+       # if the f_prime on the midpoint is less than 0,
+       # the minimizer must be on the left side of midpoint.
+       int[2] <- midpoint
+       midpoint <- (int[1]+int[2]) /2
+     } else
+       if(f_prime_a == 0)
+       {
+         break
+       }
+     # ::: FILL IN CODE HERE (UPDATE)
+     f_prime_a <- f_prime(midpoint)
+   }
+   int
+   print(paste0("Iteration for ",N," times;",
+               " The maximum value is at ", round(int[1],6)))
+ }

```

3.3 The Newton's Method

More information about this method can be found on *Page 116* of Chong and Zak (2013).

```

> newton <- function(f_prime, f_dbl, precision = 1e-6, start)
+ {
+   x_old <- start
+   x_new <- x_old - f_prime(x_old)/f_dbl(x_old)
+
+   i <- 1
+   print(paste0("Iteration ", i, "; Estimate = ", x_new) )
+   while (abs(x_new-x_old) > precision){
+     x_old <- x_new
+     x_new <- x_old - f_prime(x_old)/f_dbl(x_old)
+     # ::: redefine variables and calculate new estimate
+     # ::: keep track of iteration history
+     print(paste0("Iteration ", i+1, "; Estimate = ", x_new) )
+     i <- i + 1
+   }
+   x_new
+ }

```

Q4:

Apply each of the three functions to this example to discover the minimum. Keep track of and report the number of iterations required for each method. Report the coordinates of the minimum discovered by each of the three functions as well as the number of iterations required

MY SOLUTION:

4.1 Apply the Golden Section Search

```
> golden(f_neg, c(0,4))
[1] "Iteration for 32 times; The maximum value is at0.368352"
```

4.2 Apply the Bisection Method

```
> bisection(f_prime_neg, c(0,4))
[1] "Iteration for 26 times; The maximum value is at 0.368352"
```

4.3 Apply the Newton's Method

First, I need to get the second derivative of the original function. Based on the Quotient Rule and Chain Rule, one can easily have

$$f(x)'' = -6x^2 - 2 - \frac{2}{9}x^{-\frac{5}{3}}$$

```
> # write the second derivative function
> f_dbl <- function(x){
+   out_ <- -6*x^2-2-(2/9)*x^(-5/3)
+   return(out_)
+ }
> # since this question requires the maximum, I use -1 times the function.
> f_dbl_neg <- function(x){
+   out_ <- -6*x^2-2-(2/9)*x^(-5/3)
+   return(out_*(-1))
+ }
```

Plug the first and the second derivatives into the Newton's Method function.

```
> newton(f_prime_neg, f_dbl_neg, start = 1)
[1] "Iteration 1; Estimate = 0.918918918918919"
[1] "Iteration 2; Estimate = 0.830999851550479"
[1] "Iteration 3; Estimate = 0.736988742573808"
[1] "Iteration 4; Estimate = 0.639870150729756"
[1] "Iteration 5; Estimate = 0.546642635261104"
[1] "Iteration 6; Estimate = 0.468667930513546"
[1] "Iteration 7; Estimate = 0.416016821629135"
[1] "Iteration 8; Estimate = 0.388211559563474"
[1] "Iteration 9; Estimate = 0.376060038291039"
[1] "Iteration 10; Estimate = 0.371254711645403"
[1] "Iteration 11; Estimate = 0.369432581306114"
[1] "Iteration 12; Estimate = 0.368752709077139"
[1] "Iteration 13; Estimate = 0.368500562445562"
[1] "Iteration 14; Estimate = 0.368407257199536"
[1] "Iteration 15; Estimate = 0.368372758807196"
[1] "Iteration 16; Estimate = 0.36836000738855"
[1] "Iteration 17; Estimate = 0.368355294697857"
[1] "Iteration 18; Estimate = 0.36835355304667"
[1] "Iteration 19; Estimate = 0.368352909401224"
[1] 0.3683529
```

All three methods have the identical results, that is the maximum point of the given function is at $x = .368352$, as shown in **Figure.1**. As for the iteration times at the x interval $[0, 4]$, the Golden Section Search iterated 32 times; the Bisection Method iterated 26 times. However, Newton's method iteration time largely depends on the start numbers. That is, the more guessing number close to the target, the less times needed.

Q5:

Did the methods perform as you expected in terms of the number of iterations? Why or why not?

MY SOLUTION:

Yes. The bisection method has larger "step" than golden search method, therefore, the search iteration should be more efficient for bisection method. However, Newton's method iteration time largely depends on the start numbers. That is, the more guessing number close to the target, the less times needed.

Q6:

Use function `persp3d()` in package `rgl` to plot function f on $[-3,3]$...

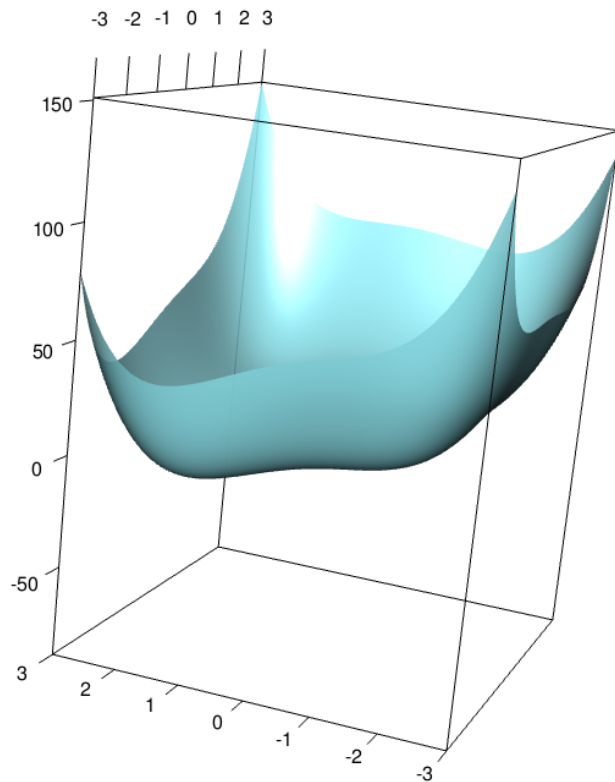
MY SOLUTION:

I write the function first.

```
> # write the function
> f_bi <- function(x_1, x_2){
+   out_ <- x_1^4 + x_2^4 - 2*x_1^2 + 2*x_1*x_2 - 3*x_2^2 + 6*x_1 - 4*x_2 + 10
+   return(out_)
+ }
```

Then, plot the 3-d surface of function.

```
> library(rgl)
> # Define grid for plotting
> x = seq(-3, 3, by = .05)
> y = seq(-3, 3, by = .05)
> xy <- expand.grid(x,y)
>
> # Calculate height of function
> # xy[,1] is vector of 'x' values; xy[,2] is vector of 'y' values
> z <- mapply(FUN = f_bi, xy[,1], xy[,2])
>
> ### Plot the surface over the domain
> plot3d(xy[,1], xy[,2], z, type = "n", radius = 1.5,
+       col = "cadetblue1", zlim = c(-90, 90), xlab = "",
+       ylab = "", zlab = "")
> surface3d(x, y, z = matrix(z,length(x)), col = "cadetblue1",
+       zlim = c(-90, 90), alpha = .9)
> knitr::include_graphics("plot-3d.png")
```



From the 3D plot, I guess the minimum point is around $(-2.1, 1.8, -11)$.

Q7:

Find the partial derivatives of f with respect to x_1 and x_2 and write a function called `grad_f()` that gives the gradient of f .

MY SOLUTION:

```
> # write the original function
> f_origin <- function(x_1, x_2){
+   out_ <- x_1^4+x_2^4-2*x_1^2+2*x_1*x_2-3*x_2^2+6*x_1-4*x_2+10
+   return(out_)
+ }
>
> # write the two partial derivatives
> dfdx_1 <- function(x_1, x_2){
+   return(4*x_1^3-4*x_1 + 2*x_2+6)
+ }
> dfdx_2 <- function(x_1, x_2){
+   return(4*x_2^3+2*x_1-6*x_2-4)
+ }
>
> # write the gradient descent function
> grad_f <- function(x_1, x_2){c(dfdx_1(x_1,x_2), dfdx_2(x_1,x_2))}
```

Q8:

Write a function to implement gradient ascent with arguments for the start point, the number of iterations, the step size α ...

MY SOLUTION:

Here, we need to discuss about the necessity of normalized gradient. Intuitively, if each time we normalize the gradient, the length of “step size” for updating is fixed. That is, the value of $Learning_Rate * Gradient's_Unit_Vector$. Apparently, it is a fixed rather than dynamic value to update the x_1 and x_2 coordination. Therefore, one can easily see the final steps will always oscillate around the target point and the stop criterion might never be reached! I choose to skip the `normalize` step, and use the $Learning_Rate * Gradient$ directly as a dynamic updating value to avoid the oscillation. That is, the closer to the target point, the smaller the step size.

```
> gradient_d <- function(f_original, # the original function
+                         grad_f, # the gradient function
+                         start_point, # the start point, a vector
+                         max_iter=100, # the maximum number of iteration
+                         alpha=0.03, # learning rate/ step size
+                         epsilon=1e-5 # stopping criterion
+ ){
+   # initial settings
+   p_old <- start_point; i <- 1; check <- 1
+   while (check > epsilon) {
+     # print the iteration information at each 10 rounds
+     # if (i == 1 | i%%5 == 0){
+     #   print(paste0("Iter ", i, "; f(x_1, x_2)= ", f_original(p_old[1], p_old[2])))}
+     print(paste0("Iter ", i, "; f(x_1, x_2)= ", f_original(p_old[1], p_old[2])))
+     # Stop condition and warning
+     if (i > max_iter) {
+       print("Exceed maximum number of iterations")
+       break
+     }
+     if (abs(p_old[1]) > 3 | abs(p_old[2] > 3)) {
+       print("Exceed the Given Range")
+       break
+     }
+     # load the gradient
+     gradient_ <- grad_f(p_old[1], p_old[2])
+     # As discussed above, I choose to not use the normalized gradient here
+     # gradient_norm <- gradient_/sqrt(gradient_**gradient_)
+     # update the point coordination with gradient * learning rate
+     p_new <- p_old - alpha*gradient_
+     # check the updating rate of p_new, if less than epsilon, stop
+     check <- sqrt((p_new-p_old)**(p_new-p_old))/ sqrt(p_old ** p_old)
+     # redefine the old point to send for next updating
+     p_old <- p_new
+     i <- i + 1
+   }
+   print(paste0("The minimum point is around ",
+               round(p_old[1],4), " ",
+               round(p_old[2],4), " ",
+               round(f_original(p_old[1],p_old[2]),4)))
+ }
```


Then, try this gradient descent method on the given function.

```
> gradient_d(f_origin, grad_f, c(1,2))
[1] "Iter 1; f(x_1, x_2)= 15"
[1] "Iter 2; f(x_1, x_2)= 7.81301856"
[1] "Iter 3; f(x_1, x_2)= 6.13673240489959"
[1] "Iter 4; f(x_1, x_2)= 4.45179110852303"
[1] "Iter 5; f(x_1, x_2)= 2.46623606070743"
[1] "Iter 6; f(x_1, x_2)= -0.020016603013886"
[1] "Iter 7; f(x_1, x_2)= -3.06809730294683"
[1] "Iter 8; f(x_1, x_2)= -6.35515915651194"
[1] "Iter 9; f(x_1, x_2)= -9.0349641871389"
[1] "Iter 10; f(x_1, x_2)= -10.4007619836912"
[1] "Iter 11; f(x_1, x_2)= -10.7691610996711"
[1] "Iter 12; f(x_1, x_2)= -10.8215165666176"
[1] "Iter 13; f(x_1, x_2)= -10.8265520327193"
[1] "Iter 14; f(x_1, x_2)= -10.826987724242"
[1] "Iter 15; f(x_1, x_2)= -10.8270254054114"
[1] "Iter 16; f(x_1, x_2)= -10.8270286959674"
[1] "Iter 17; f(x_1, x_2)= -10.8270289848232"
[1] "Iter 18; f(x_1, x_2)= -10.8270290102356"
[1] "The minimum point is around -1.5711 1.6143 -10.827"
```

For text space concern, I choose to print the iteration information at each 10 rounds. The final result shows that the minimum point is around $(-1.5711, 1.6143, -10.827)$, which is close to the observed possible minimum point $(-2.1, 1.8, -11)$ (in my response to Question 6).

Q9:

Discuss what changes would need to be made to the gradient ascent function to implement steepest ascent. You do not need to actually implement steepest ascent here but you can do so for bonus points.

MY SOLUTION:

To find the steepest “step” for updating, we need to introduce the adaptive learning rate α . I write my intuitive understanding here. Since space over 3 dimensions is hard to imagine, I take the 3-d space for discussion with the function of $f(x_1, x_2)$. In this space, any pair of x_1, x_2 can construct a plane at the height of $f(x_1, x_2)$. To find the best learning rate at the point x_1, x_2 is to find the best direction that minimizes the $f(x'_1, x'_2) - f(x_1, x_2)$. Why minimizes? At vertical direction, the steepest direction occurs at the orthogonal distance between two planes. In other words, the orthogonal distance is the minimum value of $f(x_k - \alpha * \nabla f(x_k))$, like discussed in Prof. Keller’s in-class notes. Based on this principle, I refer to and fine-tune the code that Prof. Keller provided in the notes. Note, I **insist** to use the non-normalized gradient directly to avoid the oscillation (non-convergence), as discussed in my response to Q8.

Finally, the iteration time for the steepest descent method is 8, much less than the previous method with 18 iterations.

```
> gradient_dynamic <-
+   function(f_original, # the original function
+           grad_f, # the gradient function
+           start_point, # the start point, a vector
+           max_iter=500, # the maximum number of iteration
+           alpha=0.03, # learning rate/ step size
+           epsilon=1e-5, # stopping criterion
+           minimize=TRUE
```

```

+ ){
+   # initial settings
+   p_old <- start_point; i <- 1; check <- 1
+   while (check > epsilon) {
+     # print the iteration information at each 10 rounds
+     # if (i == 1 | i%%5 == 0){
+     #   print(paste0("Iter ", i, "; f(x_1, x_2)= ", f_original(p_old[1], p_old[2])))}
+     print(paste0("Iter ", i, "; f(x_1, x_2)= ", f_original(p_old[1], p_old[2])))
+     # Stop condition and warning
+     if (i > max_iter) {
+       print("Exceed maximum number of iterations")
+       break
+     }
+     if (abs(p_old[1]) > 3 | abs(p_old[2] > 3)) {
+       print("Exceed the Given Range")
+       break
+     }
+     # load the gradient
+     gradient_ <- grad_f(p_old[1], p_old[2])
+     # As discussed above, I choose to not use the normalized gradient here
+     # gradient_norm <- gradient_/sqrt(gradient_%*%gradient_)
+     # -----Add the steepest descent-----
+     if(minimize) { f_min <- function(alpha) {
+       p_temp <- p_old - alpha*gradient_
+       f_original(p_temp[1], p_temp[2]) }
+       alpha <- optimize(f_min, interval = c(0, 1), maximum = FALSE)$minimum
+       # update the point coordination with gradient * learning rate
+       p_new <- p_old - alpha*gradient_
+     } else { f_max <- function(alpha) {
+       p_temp <- p_old - alpha*gradient_
+       f_original(p_temp[1], p_temp[2]) }
+       alpha <- optimize(f_max, interval = c(0, 1), maximum = TRUE)$maximum
+       p_new <- p_old - alpha*gradient_
+     }
+     # check the updating rate of p_new, if less than epsilong, stop
+     check <- sqrt((p_new-p_old)%*%(p_new-p_old))/ sqrt(p_old %*% p_old)
+     # redefine the old point to send for next updating
+     p_old <- p_new
+     i <- i + 1
+   }
+   print(paste0("The minimum point is around ",
+     round(p_old[1],4)," ",
+     round(p_old[2],4)," ",
+     round(f_original(p_old[1],p_old[2]),4)))
+ }
+
>
> gradient_dynamic(f_origin, grad_f, c(1,2), minimize = T)
[1] "Iter 1; f(x_1, x_2)= 15"
[1] "Iter 2; f(x_1, x_2)= 8.63699144697386"
[1] "Iter 3; f(x_1, x_2)= 4.33384987750813"
[1] "Iter 4; f(x_1, x_2)= -2.3058502980118"
[1] "Iter 5; f(x_1, x_2)= -10.6316001267316"
[1] "Iter 6; f(x_1, x_2)= -10.8270249705974"
[1] "Iter 7; f(x_1, x_2)= -10.8270290033752"

```

```
[1] "Iter 8; f(x_1, x_2)= -10.8270290126678"  
[1] "The minimum point is around -1.5711 1.6143 -10.827"
```

Reference

This homework is finished by Chenguang Pan and Seng Lei with enthusiasm for statistical learning methods. We refer to Prof. Keller's in-class note and the text book. No AI assistance is used at all. Thank you for your time.