Homework on Newton's methods

Minghe Wang, mw3845

Problem 1: Univariate optimizations.

In this problem, you will compare three common methods for univariate minimization:Newton's Method, Bisection Method and Golden-Section Search.

Function A:

$$f_1(x) = \ln(1 + x^2) + x^2$$

Function B:

$$f_2(x) = x^4 - 6x^2 + 4x + 8$$

Answer the following questions:

1. Computer $f'(x)$ and $f''(x)$
2. Are $f_1(x)$ and $f_2(x)$ unimodal functions? If not, how many modes it contains?
3. Implementing Bisection, Golden Search and Newtown's methods to find global minimum of $f_1(x)$ and $f_2(x)$
4. Discuss your results – which method is fastest in terms of iteration counts? which method is easist to apply if you only know a broad interval containing the mininum? which method fails or converges poorly if started badly? how the shape of the function influences the performance of these algorithms?
5. Please show all relevant R code for bisection, golden-section, and Newton's methods.

Answer:

```
# 2.
# install.packages("rootSolve")
library(rootSolve)

f1 <- function(x) log(1 + x^2) + x^2
f1_first <- function(x) (2*x)/(1 + x^2) + 2*x
f1_second <- function(x) 2*(x^4 + x^2 + 2) / (1 + x^2)^2

f2 <- function(x) x^4 - 6*x^2 + 4*x + 8
f2_first <- function(x) 4*x^3 - 12*x + 4
f2_second <- function(x) 12*x^2 - 12
critical_points_f2 <- uniroot.all(f2_first, lower = -10, upper = 10)

# 3. find local minimum
# bisection
```

```r
# we need dfa * dfb < 0
bisection <- function(df, a, b, tol = 1e-10){
  cur <- (a + b) / 2
  i <- 0
  while (abs(df(cur)) > tol){
    i <- i + 1
    if (df(a) * df(cur) > 0){
      a <- cur
    }else {
      b <- cur
    }
    cur <- (a + b) / 2
  }
  res <- c(cur, i)
  return(res)
}

# golden search
goldenSearch <- function(f, a, b, tol=1e-10){
  gr <- (sqrt(5) - 1) / 2
  x1 <- b - gr * (b - a)
  x2 <- a + gr * (b - a)
  i <- 0
  while(abs(b - a) > tol){
    i <- i + 1
    if (f(x1) < f(x2)){
      b <- x2
      x2 <- a + gr * (b - a) # can also be x1
      x1 <- b - gr * (b - a)
    }else{
      a <- x1
      x1 <- b - gr * (b - a) # can also be x2
      x2 <- a + gr * (b - a)
    }
  }
  res <- c((a + b) / 2, i)
  return (res)
}

# newton method
newtonMethod <- function(f, df, start, tol=1e-10){
  i <- 0
  x <- start
  while (abs(f(x)) > tol){
    i <- i + 1
    x <- x - f(x) / df(x)
  }
  res <- c(x, i)
  return(res)
}
set.seed(123)
# f1
a <- -2
```

```r
b <- 1
res_f1_bisec <- bisection(f1_first, a, b)
res_f1_gs <- goldenSearch(f1, a, b)
res_f1_nt <- newtonMethod(f1_first, f1_second, a)

# f2
as <- c(-2, 0.9)
bs <- c(0, 2)
res_f2_bisec1 <- bisection(f2_first, as[1], bs[1])
res_f2_bisec2 <- bisection(f2_first, as[2], bs[2])

res_f2_gs1 <- goldenSearch(f2, as[1], bs[1])
res_f2_gs2 <- goldenSearch(f2, as[2], bs[2])

res_f2_nt1 <- newtonMethod(f2_first, f2_second, as[1])
res_f2_nt2 <- newtonMethod(f2_first, f2_second, as[2])

# 4.
comparison1 <- as.data.frame(rbind(c("bisection", res_f1_bisec, f1(res_f1_bisec[1])),
                                   c("golden search", res_f1_gs, f1(res_f1_gs[1])),
                                   c("newton method", res_f1_nt, f1(res_f1_nt[1]))))
comparison1 <- comparison1 %>%
  rename(name = "V1", root = "V2", iteration = "V3", result = "V4")
comparison1
```

```
##            name                  root iteration                result
## 1     bisection  1.45519152283669e-11        35  2.11758236813575e-22
## 2 golden search -5.79591141089835e-12        51  3.35925890829817e-23
## 3 newton method  4.58039842491341e-16         5  2.09800497309492e-31
```

```r
comparison2 <- as.data.frame(rbind(c("bisection root 1", res_f2_bisec1, f2(res_f2_bisec1[1])),
                                   c("bisection root 2", res_f2_bisec2, f2(res_f2_bisec2[1])),
                                   c("golden search root 1", res_f2_gs1, f2(res_f2_gs1[1])),
                                   c("golden search root 2", res_f2_gs2, f2(res_f2_gs2[1])),
                                   c("newton method root 1", res_f2_nt1, f2(res_f2_nt1[1])),
                                   c("newton method root 2", res_f2_nt2, f2(res_f2_nt2[1]))))
comparison2 <- comparison2 %>%
  rename(name = "V1", root = "V2", iteration = "V3", result = "V4")
comparison2
```

```
##                   name              root iteration            result
## 1     bisection root 1 -1.87938524156925        35 -8.23442238342932
## 2     bisection root 2  1.53208888624067        35  5.55437759271229
## 3 golden search root 1 -1.87938523016814        50 -8.23442238342932
## 4 golden search root 2  1.53208889529803        49  5.55437759271229
## 5 newton method root 1 -1.87938524157182         4 -8.23442238342932
## 6 newton method root 2  1.53208888623796         7  5.55437759271229
```

1.

function A: $f_1'(x) = \frac{2x}{1+x^2} + 2x$, $f_1''(x) = \frac{2(x^4+x^2+2)}{(1+x^2)^2}$

function B: $f_2'(x) = 4x^3 - 12x + 4$, $f_2''(x) = 12x^2 - 12$

2.

To find whether functions are unimodal, we need to find root where first prime of function is 0 and second prime of function is positive.

For **function A**, it is obvious that the first derivative of function is 0 only when x = 0, and $f_2''(0) = 4 > 0$. Therefore, function A is unimodal.

For **function B**, we use `library(rootSolve)` and find 3 root for function B. is not unimodal.

3.

The comparison of results for function A and B are presented above in tables.

With result from question 2, we know that root of function B are: -1.8794479, 0.3472831, 1.5320901, and their second derivatives are 30.3878946, -10.5527331, 16.1676027. Therefore, we only have 2 local minimum.

4.

According to the comparison tables, we first verify that the root of f1 is at 0 and the global minimum can also be considered as $f(0) = 0$. For f2, we wisely choose the range and starting point in order to handle its multi-modal. And by comparison, we find the global minimum of f2 is -8.2344224 at root = -1.8793852. All methods agrees with the global minimum for both functions, which indicate our estimation of global minimum is valid.

The newton's method is fastest in terms of iteration.

I think the Golden Search is the easiest method to apply if we only know a broad range because we don't need to know the expression of derivatives of function. Also, bisection and newton methods are root finding methods, but for golden search, we can implement it to obtain either maximum or minimum.

Newton's Method is most prone to failure or poor convergence when initial guess is bad. if initial guess is too far or its second derivative is too close to 0, then the method might diverge to another search region or crash(denominator=0).

Shape of function influences:

- Bisection because it requires the signs of first derivative of the range we choose to be different. Therefore, if we don't properly choose the interval, other critical points might be included.
- Golden Search because it assumes unimodality of our function. If there is multiple modals, we need to isolate each of them.
- Newton Method because the second derivative of the function(local curvature) can influence convergence significantly.

Problem 2: Newton's Method in Two Dimensions

$g(x, y)$ is a 2D funciton

$$g(x, y) = x^2 + xy + y^2 - 4x - 3y + 7$$

Answer the folling questions:

1. Derive the gradient $\Delta g(x, y)$ and the Hessian matrix $\Delta^2 g(x, y)$.
2. Implementation a Newton's algorithm to find its minimizer.
3. Choose two different starting values, and compare the resulting solutions, iteration counts and path to convergence
4. Create a coutour plot of g around its minium, and overlay the sequence of iterates from Newton's method to show the path to the minimum.

Answer: your answer starts here...

1. $\Delta g(x,y) = \binom{2x+y-4}{x+2y-3}$, $\Delta^2 g(x,y) = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$

```
# 2.
set.seed(123)
grad <- function(x, y) {
  c(2*x + y - 4,  x + 2*y - 3)
}
hess <- matrix(c(2, 1,
                 1, 2), nrow = 2, byrow = TRUE)
newtonRalphson <- function(x0, y0, grad, hess, tol=1e-10, max_iter=500){
  i <- 0
  x <- x0
  y <- y0
  hess_inv <- solve(hess)
  g_val <- grad(x, y)
  res <- c(x, y, g_val, i)
  prev_x <- -Inf
  prev_y <- -Inf
  while(i < max_iter && (x-prev_x > tol) && (y-prev_y > tol)){#sqrt(sum(g_val^2)) > tol){
    i <- i + 1
    curr <- hess_inv %*% g_val
    prev_x <- x
    prev_y <- y
    x <- x - curr[1]
    y <- y - curr[2]
    g_val <- grad(x, y)
    res <- rbind(res, c(x, y, g_val, i))
  }
  return(res)
}

res_table1 <- newtonRalphson(0.8, 0.7, grad, hess)
res_table2 <- newtonRalphson(10, -5, grad, hess)

res_table1
```

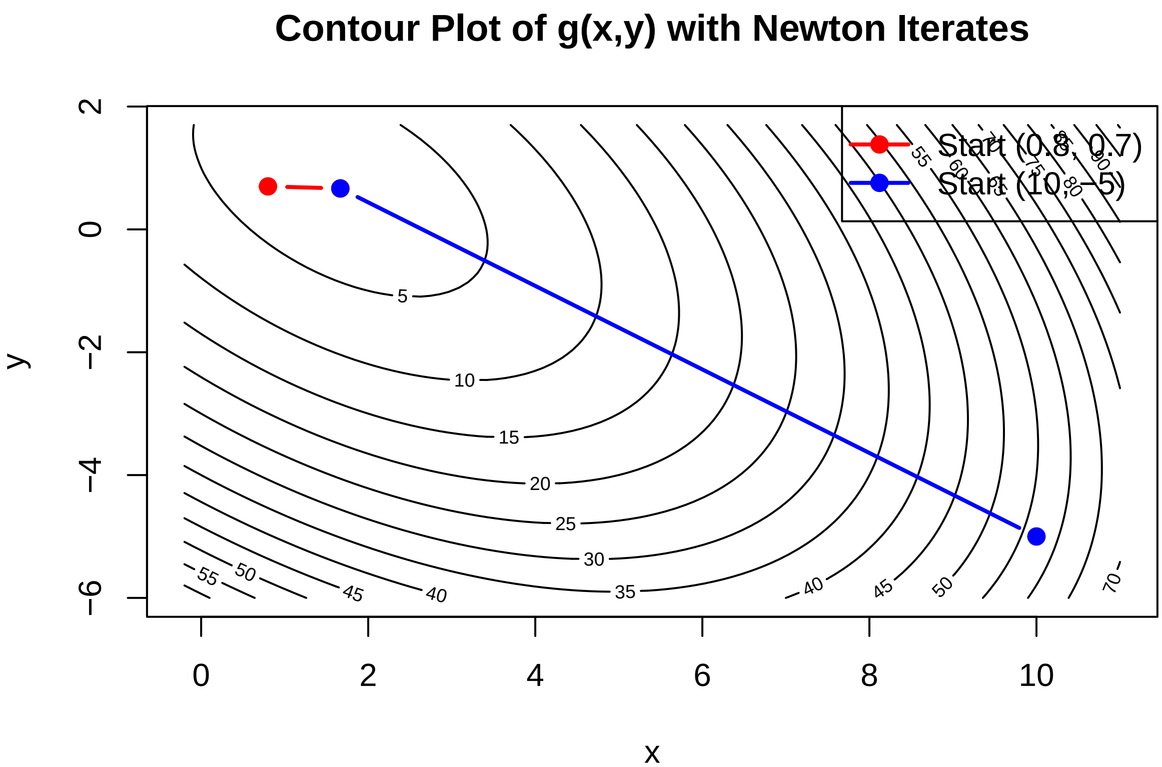
```
##         [,1]      [,2] [,3] [,4] [,5]
## res 0.800000 0.7000000 -1.7 -0.8    0
##     1.666667 0.6666667  0.0  0.0    1
```

```
res_table2
```

```
##          [,1]       [,2]         [,3] [,4] [,5]
## res 10.000000 -5.0000000 1.100000e+01   -3    0
##      1.666667  0.6666667 1.776357e-15    0    1
```

```
g <- function(x, y) {
  x^2 + x*y + y^2 - 4*x - 3*y + 7
}

all_x <- c(res_table1[,1], res_table2[,1])
all_y <- c(res_table1[,2], res_table2[,2])
x_range <- range(all_x)
```

```r
y_range <- range(all_y)
x_vals <- seq(x_range[1] - 1, x_range[2] + 1, length.out = 100)
y_vals <- seq(y_range[1] - 1, y_range[2] + 1, length.out = 100)

# Compute the function values on the grid.
z_vals <- outer(x_vals, y_vals, g)

# Plot the contour
contour(x_vals, y_vals, z_vals, nlevels = 20,
        xlab = "x", ylab = "y",
        main = "Contour Plot of g(x,y) with Newton Iterates")

lines(res_table1[,1], res_table1[,2], type = "b", col = "red", pch = 19, lwd = 2)
points(res_table1[,1], res_table1[,2], col = "red", pch = 19)

lines(res_table2[,1], res_table2[,2], type = "b", col = "blue", pch = 19, lwd = 2)
points(res_table2[,1], res_table2[,2], col = "blue", pch = 19)

# Add a legend
legend("topright", legend = c("Start (0.8, 0.7)", "Start (10, -5)"),
       col = c("red", "blue"), pch = 19, lwd = 2)
```



Problem 3

Suppose we have data $(x_i, y_i), i = 1, ..., n$, with y_i follows a conditional expotential distribution

$$Y_i \mid x_i \sim \exp(\lambda_i), \text{ where } \log(\lambda_i) = \alpha + \beta x_i.$$

Please complete the following tasks:

1. Derive the log-likelihood of (x_i, y_i), as well as its Gradient and Hession Matrix
2. Generate a syntheic data with true $\alpha = 0.5$, true $\beta = 1.2$ and sample size $n = 200$.
3. Implement an Newton's algorthm to its MLE
4. Implement a modified Newton's algorithm, where you incoporate both of the step-having and ascent direction check. If a direction is not ascent, you can swith to a simpler gradient descent.
5. For a generalized linear models, one can replace the observed Hessian with the expected Hessian (the Fisher information), which might lead to stable updates akin to a Fisher scoring approach. Implement another modified newton's algorithm with Fisher scoring toestimate MLE.
6. Compare the final parameter estimates, iteration counts and convergences of optimization, and summarize your findings.

Answer:

1. Since the conditional distribution is exponential, we use its pdf and then we have $l(\alpha, \beta) = ln \prod_{i=1}^{n} [\lambda_i] e^{-\lambda_i y_i} = \sum_{i=1}^{n} [ln(\lambda_i) - \lambda_i y_i] = \sum_{i=1}^{n} [\alpha + \beta x_i - y_i e^{\alpha + \beta x_i}]$

Gradient: $\nabla L(\alpha, \beta) = \begin{pmatrix} n - \sum_{i=1}^{n} y_i \, e^{\alpha+\beta x_i} \\ \sum_{i=1}^{n} x_i \; - \; \sum_{i=1}^{n} \big(x_i \, y_i \, e^{\alpha+\beta x_i}\big) \end{pmatrix}$.

Hessian: $\nabla^2 L(\alpha, \beta) = \begin{pmatrix} -\sum_{i=1}^{n} y_i \, e^{\alpha+\beta x_i} & -\sum_{i=1}^{n} x_i \, y_i \, e^{\alpha+\beta x_i} \\ -\sum_{i=1}^{n} x_i \, y_i \, e^{\alpha+\beta x_i} & -\sum_{i=1}^{n} x_i^2 \, y_i \, e^{\alpha+\beta x_i} \end{pmatrix}$.

```r
# 2
n <- 200
alpha_true <- 0.5
beta_true  <- 1.2
set.seed(123)
x <- runif(n, 0, 1)
# Generate predictor values (x_i)
lambda <- exp(alpha_true + beta_true * x)

# Generate y_i ~ Exp(rate = lambda_i)
y <- rexp(n, rate = lambda)

df <- data.frame(x = x, y = y)

# 3. Newton method for MLE of conditional dist
loglik_expreg <- function(alpha, beta, x, y){
  lambda <- exp(alpha + beta * x)
  val <- sum((alpha + beta * x) - y * lambda)
  return (val)
}

grad_expreg <- function(alpha, beta, x, y) {
  lambda <- exp(alpha + beta * x)
  d_alpha <- length(x) - sum(y * lambda)
  d_beta  <- sum(x) - sum(x * y * lambda)
  return(c(d_alpha, d_beta))  # 2x1 vector
}
```

```r
hess_expreg <- function(alpha, beta, x, y) {
  lambda <- exp(alpha + beta * x)
  term   <- y * lambda  # common term y_i e^{alpha+beta x_i}

  h11 <- -sum(term)            # d^2/dalpha^2
  h22 <- -sum(x^2 * term)      # d^2/dbeta^2
  h12 <- -sum(x * term)        # d^2/dalpha dbeta = d^2/dbeta dalpha
  H <- matrix(c(h11, h12,
                 h12, h22),
               nrow = 2, byrow = TRUE)
  return(H)
}

newton_expreg <- function(x, y, alpha_init = 0, beta_init = 0,
                          tol = 1e-8, max_iter = 100) {
  alpha <- alpha_init
  beta <- beta_init
  i <- 0
  prev_loglik <- -Inf
  curr_loglik <- loglik_expreg(alpha, beta, x, y)

  while (i < max_iter && abs(curr_loglik - prev_loglik) > tol) { # or compute gradient norm sqrt(sum(g^
    i <- i+1
    g <- grad_expreg(alpha, beta, x, y)
    H <- hess_expreg(alpha, beta, x, y)

    # Update alpha, beta via Newton step
    update <- solve(H, g)  # H^{-1} * g
    alpha <- alpha - update[1]
    beta  <- beta  - update[2]

    # Update log-likelihood
    prev_loglik <- curr_loglik
    curr_loglik <- loglik_expreg(alpha, beta, x, y)
  }
  return (list(alpha = alpha,
               beta   = beta,
               loglik = curr_loglik,
               iter = i))
}

res_newtonRalphson <- newton_expreg(x, y,
                           alpha_init = 0, beta_init = 0,
                           tol = 1e-10, max_iter = 200)

# 4. step halving at the end when ascent direction
modified_newton_expreg <- function(x, y,
                                   alpha_init = 0,
                                   beta_init  = 0,
                                   tol = 1e-8,
                                   max_iter = 100) {

  alpha <- alpha_init
```

```r
beta  <- beta_init
i     <- 0

prev_loglik <- -Inf
curr_loglik <- loglik_expreg(alpha, beta, x, y)

while (i < max_iter && abs(curr_loglik - prev_loglik) > tol) {
  i <- i + 1

  # Compute gradient and Hessian
  g <- grad_expreg(alpha, beta, x, y)    # a 2-vector
  H <- hess_expreg(alpha, beta, x, y)    # a 2x2 matrix

  # Newton update is effectively -H^-1 * g
  update <- solve(H, g)                  # H^-1 g
  # The "Newton direction" in terms of "move" is -update:
  d_newton <- -update

  # Check if d_newton is ascent
  dir_check <- sum(g * d_newton)
  if (dir_check <= 0) {
    # fallback: use gradient direction
    d <- g
  } else {
    d <- d_newton
  }

  # Step-halving line search
  step <- 1
  old_loglik <- curr_loglik
  # Proposed new parameters
  new_alpha <- alpha + step * d[1]
  new_beta  <- beta  + step * d[2]
  new_loglik <- loglik_expreg(new_alpha, new_beta, x, y)

  # While new log-likelihood <= old, reduce step
  while (step > 1e-14 && new_loglik <= old_loglik) {
    step <- step / 2
    new_alpha <- alpha + step * d[1]
    new_beta  <- beta  + step * d[2]
    new_loglik <- loglik_expreg(new_alpha, new_beta, x, y)
  }

  # Update alpha, beta, loglik
  prev_loglik <- curr_loglik
  alpha <- new_alpha
  beta  <- new_beta
  curr_loglik <- new_loglik
}

list(alpha = alpha,
     beta  = beta,
     loglik = curr_loglik,
```

```r
      iter = i)
}


# 5. Fisher score modified
newton_expreg_fisher <- function(x, y,
                                 alpha_init = 0, beta_init = 0,
                                 tol = 1e-8, max_iter = 100) {
  # Initialize parameters
  alpha <- alpha_init
  beta  <- beta_init
  i <- 0
  prev_loglik <- -Inf
  curr_loglik <- loglik_expreg(alpha, beta, x, y)

  while (i < max_iter && abs(curr_loglik - prev_loglik) > tol) {
    i <- i + 1
    g <- grad_expreg(alpha, beta, x, y)

    # Compute the Fisher Information matrix.
    I_mat <- matrix(c(length(x), sum(x),
                      sum(x),      sum(x^2)),
                    nrow = 2, byrow = TRUE)

    # Compute the Fisher scoring update:
    # update = I^{-1} * g. (For maximization, we add this update.)
    update <- solve(I_mat, g)


    # Step-halving (line search) to ensure an increase in log-likelihood.
    step <- 1
    old_loglik <- curr_loglik
    new_alpha <- alpha + step * update[1]
    new_beta  <- beta  + step * update[2]
    new_loglik <- loglik_expreg(new_alpha, new_beta, x, y)

    while (step > 1e-14 && new_loglik < old_loglik) {
      step <- step / 2
      new_alpha <- alpha + step * update[1]
      new_beta  <- beta  + step * update[2]
      new_loglik <- loglik_expreg(new_alpha, new_beta, x, y)
    }

    # Update the parameters and log-likelihood
    prev_loglik <- curr_loglik
    alpha <- new_alpha
    beta  <- new_beta
    curr_loglik <- new_loglik
  }

  return(list(alpha = alpha,
              beta  = beta,
              loglik = curr_loglik,
```

```r
              iter = i))
}

res_orig   <- newton_expreg(x, y, alpha_init = 0, beta_init = 0, tol = 1e-10, max_iter = 200)
res_mod    <- modified_newton_expreg(x, y, alpha_init = 0, beta_init = 0, tol = 1e-10, max_iter = 200)
res_fisher <- newton_expreg_fisher(x, y, alpha_init = 0, beta_init = 0, tol = 1e-10, max_iter = 200)

# Create a comparison table
results <- data.frame(Method = c("Original Newton", "Modified Newton", "Fisher Scoring"),
                      Alpha = c(res_orig$alpha, res_mod$alpha, res_fisher$alpha),
                      Beta  = c(res_orig$beta,  res_mod$beta,  res_fisher$beta),
                      LogLik = c(res_orig$loglik, res_mod$loglik, res_fisher$loglik),
                      Iterations = c(res_orig$iter, res_mod$iter, res_fisher$iter))

print(results)
```

```
##            Method     Alpha     Beta   LogLik Iterations
## 1 Original Newton 0.2974917 1.554776 16.96356          8
## 2 Modified Newton 0.2974917 1.554776 16.96356          5
## 3  Fisher Scoring 0.2974917 1.554776 16.96356          7
```

6. Based on the comparison table above, we found that all methods can find the MLE quickly and the modified newton ralphson with ascent check and step halving is the fastest as we expected. All three methods agrees on an optimum, which indicates our result is valid.