

# ISyE 6416 Homework 2: Optimization

## Optimization Basics and Multivariate Variables

Shixiang Zhu

Georgia Institute of Technology

Atlanta, Georgia

shixiang.zhu@gatech.edu

### ABSTRACT

In this report, we work out the problem 2.1 and problem 2.5, which focus on understanding and implementing various of optimization methods by trying on given dataset. Throughout this work, we mainly explore the methods including *Raphson Newton Method*, *Bisection Method*, *Fixed Points iteration*, *Secant Method* for univariate optimization problem, and *Newton-like Method*, *Fisher Scoring Iteration*, *Quasi-Newton Method* for multivariate optimization problem. In addition, we also try to identify how backtracking trick would impact the outcome of some optimization methods.

### KEYWORDS

optimization, multivariate, MLE

## 1 INTRODUCTION

In this work, the relevant code is attached to the end of this report as appendices. Moreover, we will further explain two problems (2.1 and 2.5) from text book and plot the experimental figures for each experiment (problem). In detail, we split our code into four files, including `main.R` in Appendix A, `rootfinder.R` in Appendix B, `optimizer.R` in Appendix C and `plotter.R` in Appendix D. `rootfinder.R` and `optimizer.R` contain all the available methods for solving optimization for univariates and multivariates respectively. `plotter.R` contains utilities for plotting all the figures in this report.

## 2 PROBLEM 2.1

The following data are an i.i.d sample from a  $Cauchy(\theta, 1)$  distribution: 1.77, -0.23, 2.76, 3.80, 3.47, 56.75, -1.34, 4.24, -2.44, 3.29, 3.71, -2.40, 4.53, -0.07, -1.05, -13.87, -2.53, -1.75, 0.27, 43.21. At first step, we would like to see how's the log likelihood function of Cauchy distribution ( $Cauchy(\theta, \sigma)$ ) look like. As shown in Fig. 1, the maximum value is located around location 0.5 and scale 0.8. When scale is fixed at 1, it turns the local maximum value of log-likelihood function shown in Fig. 2 is around 0.

As we can easily it is an univariate optimization problem, we apply Maximum likelihood estimation (MLE) to maximize the real-valued log-likelihood function  $g(x)$  of a Cauchy distribution  $Cauchy(\theta, 1)$ . Let's consider the location-scale family of Cauchy distribution whose PDFs are given by

$$f(x; \theta, \sigma) = \frac{1}{\pi\sigma} \left(1 + \left(\frac{x - \theta}{\sigma}\right)^2\right)^{-1}$$

where  $\theta$  is its location and  $\sigma$  is its scale, in our scenario, it equals to 1. By definition, the log-likelihood  $\mathcal{L}$  of a batch of sample data (shown above),  $x_i, i = 1, 2, 3, \dots, n$  is the logarithm of their probability, assuming the data are independently and identically

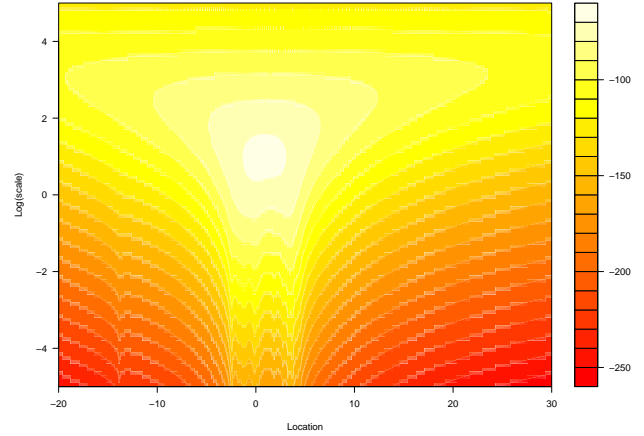


Figure 1: Loglikelihood Function of  $Cauchy(\theta, \sigma)$

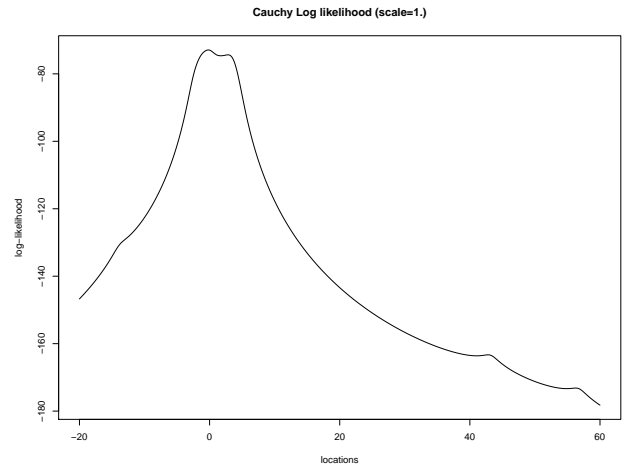


Figure 2: Loglikelihood Function of  $Cauchy(\theta, 1)$

distributed according to  $f(x; \theta, \sigma)$ . The independence assumption implies the probability is the product of individual probabilities, whence

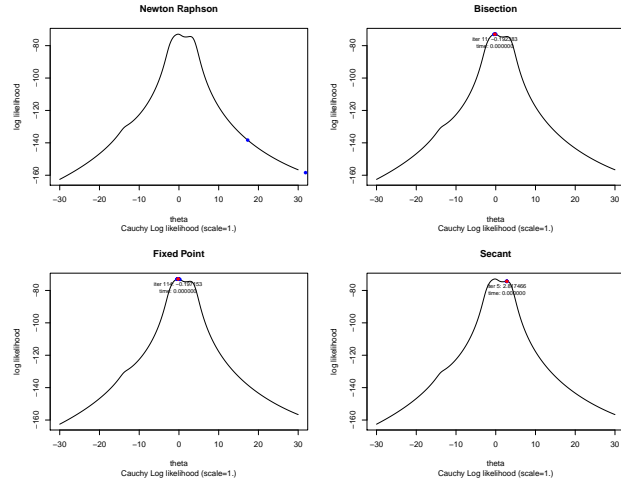


Figure 3: The solutions and iterations traces of four MLE methods on the log-likelihood.

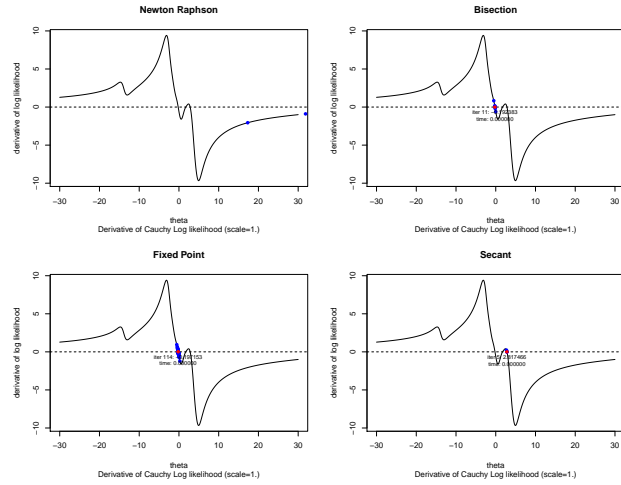


Figure 4: The solutions and iterations traces of four MLE methods on the derivative of the log-likelihood.

$$\begin{aligned}\mathcal{L}(\theta; \sigma = 1, x) &= \log \prod_{i=1}^n f(x_i; \theta, \sigma = 1) \\ &= - \sum_{i=1}^n \log \left( 1 + \left( \frac{x_i - \theta}{\sigma} \right)^2 \right) - n \log(\pi \sigma).\end{aligned}$$

In order to understand the physics behind univariate optimization better, we manually implement four methods for *Raphson Newton Method*, *Bisection Method*, *Fixed Point Iteration* and *Secant Method* respectively in *findroot.R* of Appendix B. In our **R** code, We use `numDeriv` package to solve the first derivative for our self-defined log-likelihood functions. For Problem 2.1 from (a) to (d), we plot our solutions for these four methods on the log-likelihood

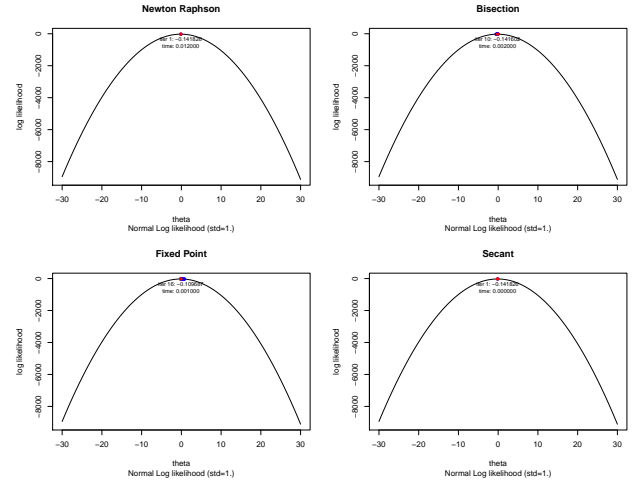


Figure 5: The solutions and iterations traces of four MLE methods on the log-likelihood.

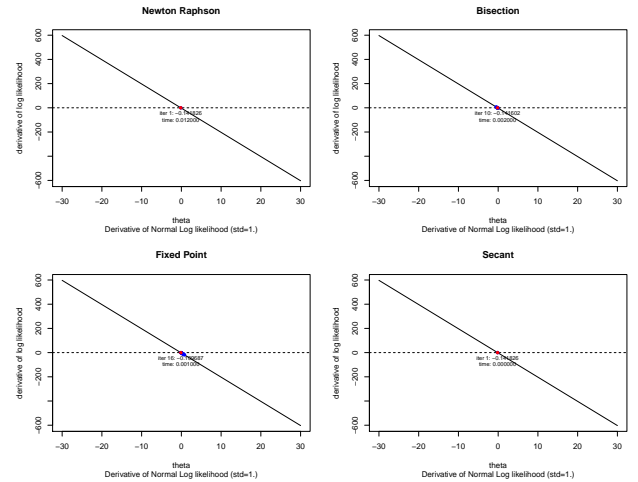


Figure 6: The solutions and iterations traces of four MLE methods on the derivative of the log-likelihood.

function of Cauchy distribution (shown in Fig. 3) and its derivatives (shown in Fig. 4) respectively.

In problem 2.1 (e), we also apply same methods to a random sample of size 20 from a  $N(\theta, 1)$  distribution by using function `rnorm` in **R**. We likewise model these randomly generated data points with MLE. The PDF of a Normal distribution is

$$f(x; \mu, \sigma) = (2\pi\sigma^2)^{-1/2} \exp\left(-\frac{1}{2} \frac{(x - \mu)^2}{\sigma^2}\right)$$

where  $\mu$  is mean and  $\sigma^2$  is variance, which are the two parameters that need to be estimated. Therefore, the log-likelihood function can be expressed as

$$\mathcal{L}(\mu; \sigma = 1, x) = -\frac{n}{2} \ln(2\pi) - \frac{n}{2} \ln(\sigma^2) - \frac{1}{2\sigma^2} \sum_{i=1}^n (x_i - \mu)^2$$

In Fig. 3, Fig. 4, Fig5 and Fig. 6 the red points mean the final solution for corresponding methods, and following a trace of blue points mean the history of iteration when finding the roots. According to the experiments, the local optimal point is highly depended on its initial choices. We can draw some same conclusions from these experiments. For example, *Fisher Scoring Iterations* generally makes rapid improvements initially, while Newton-like method gives better refinements near the end, however, sometime according to our observations, Newton-like method cannot get valid solution when the starting point is too far away from the true optimal point. Regarding *Fixed Points Iteration* usually takes more steps to get convergence. Instead, *Bisection* and *Secant* Method can get convergence within very few steps. In terms of the speed of computation, it is really hard to differentiate these four method when dealing with the log-likelihood of Cauchy, but *Secant* has an clear edge over the other three methods.

### 3 PROBLEM 2.5

In problem 2.5, there were 46 crude oil spills of at least 1,000 barrels from tankers in U.S. waters during 1974-1999. The website for this book contains the following data: the number of spills in the  $i$ -th year,  $N_i$ ; the estimated amount of oil shipped through US waters as part of US import/export operations in the  $i$ -th year, adjusted for spillage in international or foreign waters,  $b_{i1}$ ; and the amount of oil shipped through U.S. waters during domestic shipments in the  $i$ -th year,  $b_{i2}$ . The data are adapted from. Oil shipment amounts are measured in billions of barrels (Bbbl). The volume of oil shipped is measure of exposure to spill risk. Suppose we use the Poisson process assumption given by  $N_i | b_{i1}, b_{i2} \sim \text{Poisson}(\lambda_i)$  where  $\lambda_i = \alpha_1 * b_{i1} + \alpha_2 * b_{i2}$ . The parameters of this model are  $\alpha_1$  and  $\alpha_2$ , which represent the rate of spill occurrence per Bbbl oil shipped during import/expert and domestic shipments, respectively.

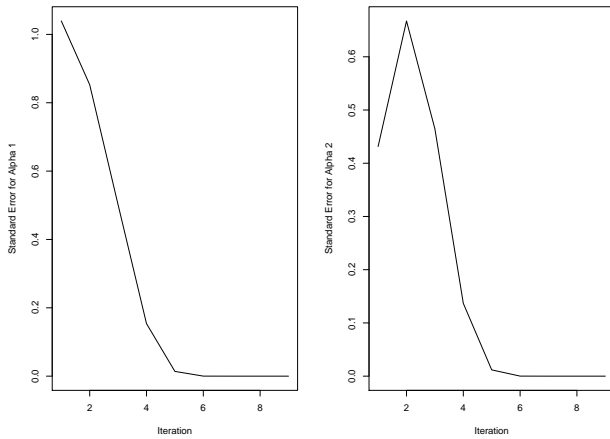


Figure 7: Standard error of  $\alpha$  over iterations.

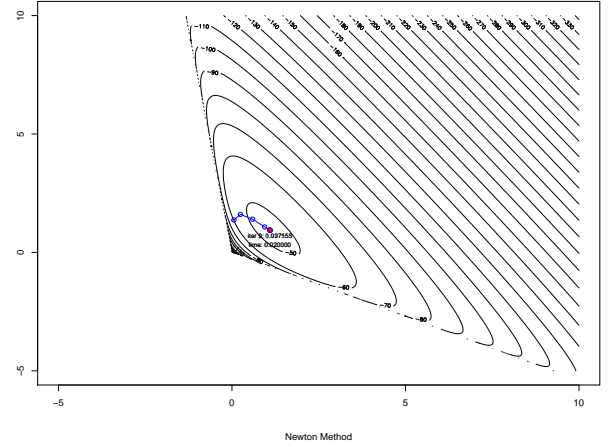


Figure 8: Newton Method.

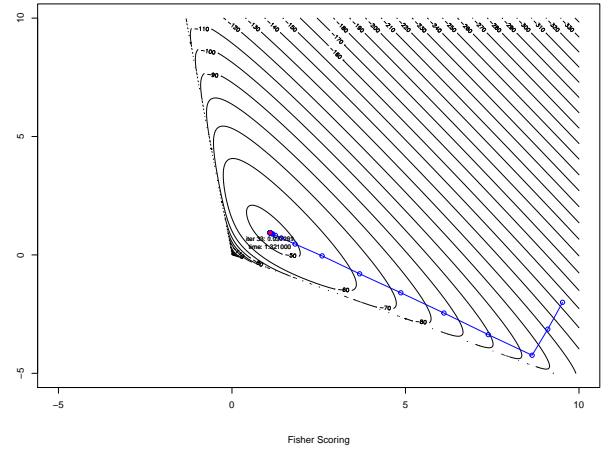


Figure 9: Fisher Scoring.

Thus, according to definition, the probability mass function of a term of the sequence  $x$  is

$$p_i(N_i) = \begin{cases} \frac{(\alpha_1 b_{i1} + \alpha_2 b_{i2})^{N_i} e^{-(\alpha_1 b_{i1} + \alpha_2 b_{i2})}}{N_i!}, & \text{if } N_i \in \mathbb{Z}_+ \\ 0, & \text{if } x \notin \mathbb{Z}_+ \end{cases}$$

And the log-likelihood function is

$$\begin{aligned} \mathcal{L}(\alpha_1, \alpha_2; N_i, b_{i1}, b_{i2}) &= -n(\alpha_1 b_{i1} + \alpha_2 b_{i2}) \\ &\quad - \sum_{i=1}^n \ln(N_i!) + \ln(\alpha_1 b_{i1} + \alpha_2 b_{i2}) \sum_{i=1}^n x_i. \end{aligned}$$

In problem 2.5 (a) to (d), we discuss about the performance of *Newton* and *Fisher Scoring* methods for multivariate estimation problem. Specifically, as shown in Fig. 8 and Fig. 9, textitNewton can only work with initial points in a very limited extent, however, *Fisher Scoring* can work with initial points even at the margin of

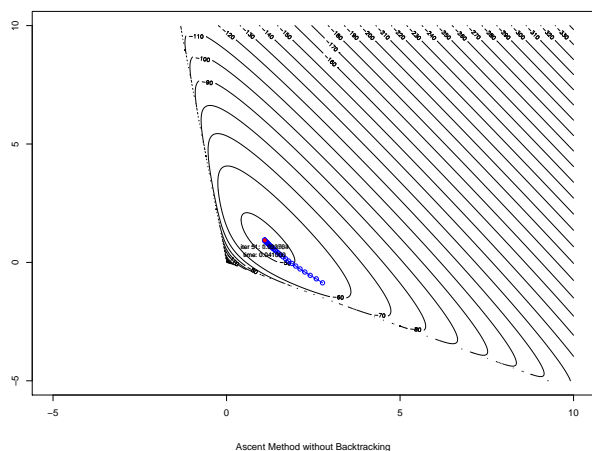


Figure 10: Steepest ascent method without backtracking.

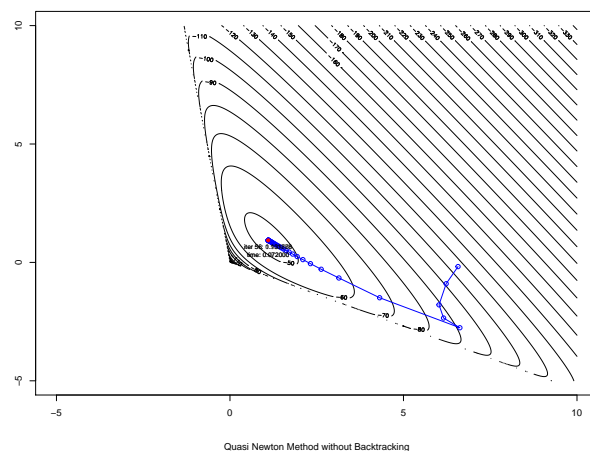


Figure 12: Quasi-Newton method without backtracking.

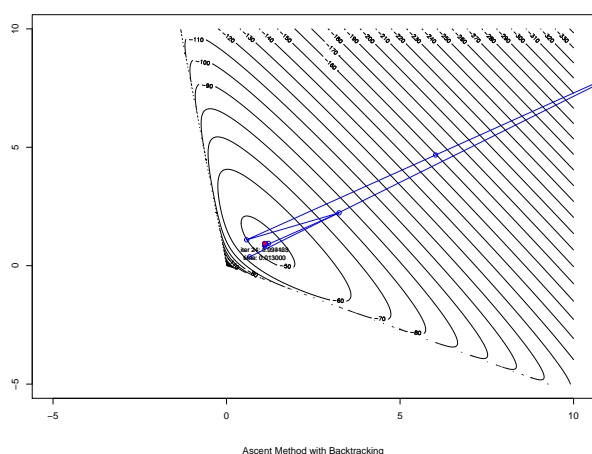


Figure 11: Steepest ascent method with backtracking.

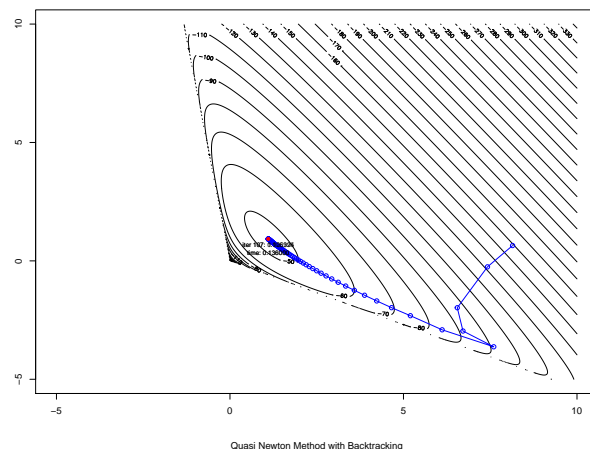


Figure 13: Quasi-Newton method with backtracking.

range in this figure. Similarly, here the red points mean the final solution of local optimal and blue points mean the trace of solutions over iterations. In Fig. 7, we also show the standard error of  $\alpha_1$  and  $\alpha_2$  over iterations in accordance with the requirement of problem 2.5 (d).

In problem 2.5 (e) and (f), we further evaluate the influences of backtracking trick when applying on *Quasi-Newton* method and *Steepest Ascent* method. Generally, backtracking trick allows the algorithm make much bolder attempts even the step is downhill. As we can easily tell in Fig. 10, Fig. 11, Fig. 12 and Fig. 13, the iteration trace of methods with backtracking look zigzag, sometimes it even make the tentative steps over the local optimal, which usually means fast convergence speed. Comparing to the iteration trace of methods without backtracking, they look smoother than the previous.

## 4 CONCLUSION

In sum, we discuss several common optimization methods in this report, and do contrast experiments for each of them. Generally, *Quasi-Newton* is the fastest method for finding local optimal, which is also the most commonly-used method for optimization (like *BFGS*). And backtracking trick can speed some algorithm up under some certain conditions.

## Appendices

### A MAIN.R APPENDIX

```
1 # HW2 - Optimization
2 # updated at Feb 5, 2018
3 # by Shixiang (Woody) Zhu
4
5 # Configurations
6 rootPath <- "your/path/to/project/"
```

```

7 dataPath <- paste(rootPath, "datasets/oilspills.dat", sep="/")
8 source(paste(rootPath, "hw2-optimization/rootfinder.R", sep="/"))
9 source(paste(rootPath, "hw2-optimization/optimizer.R", sep="/"))
10 source(paste(rootPath, "hw2-optimization/plotter.R", sep="/"))
11
12 # Problem 1:
13 # =====
14 # The following data are an i.i.d sample from a Cauchy(theta, 1) distribution:
15 data <- c(1.77, -0.23, 2.76, 3.80, 3.47, 56.75, -1.34, 4.24, -2.44, 3.29, 3.71,
16          -2.40, 4.53, -0.07, -1.05, -13.87, -2.53, -1.75, 0.27, 43.21)
17
18 # Loglikelihood function of Cauchy distribution (theta, scale=1)
19 loglikCauchy <- function(location, scale=1., xs=data) {
20   sum(dcauchy(xs, location=location, scale=scale, log=TRUE))
21 }
22
23 # Derivative of loglikelihood function of Cauchy distribution (theta, 1)
24 derivLoglikCauchy <- function(location, xs=data) {
25   2 * sum((xs - location) / (1 + (xs - location)^2))
26 }
27
28 locations <- seq(-20, 60, 1/50) # Range of medians to plot
29 scales <- seq(-5, 5, 1/50) # Range of (log) scales to plot
30 u <- as.matrix(expand.grid(locations, exp(scales))) # Points to evaluate
31 y <- apply(as.matrix(locations), 1, function(v) loglikCauchy(v, 1., data))
32 z <- matrix(apply(u, 1, function(v) loglikCauchy(v[1], v[2], data)),
33            nrow=length(locations))
34
35 # -----
36 # a. Graph the log-likelihood function as location and scale vary
37 filled.contour(locations, scales, z, color.palette=heat.colors,
38               xlab="Location", ylab="Log(scale)",
39               main="Cauchy_Log_Likelihood")
40
41 # Graph the log-likelihood function as only location vary when scale=1.
42 plot(locations, y, type="l", xlab="locations", ylab="log-likelihood",
43       main="Cauchy_Log_likelihood_(scale=1.)")
44
45 # Find the MLE for theta using the Newton-Raphson method. Try all of the
46 # following starting points:
47 startPois <- c(-11, -1, 0, 1.5, 4, 4.7, 7, 8, 38)
48 # Discuss your results. Is the mean of the data is a good starting point?
49
50 # Solve Maximum likelihood Estimation by Newton Raphson
51 newtonMLE <- newtonRaphson(f=derivLoglikCauchy, x0=mean(data))
52 # # Plot solutions on their loglikelihood function and its derivative function
53 plotSol(locations, derivLoglikCauchy, newtonMLE,
54         xlabel="theta", ylabel="derivative of log likelihood",
55         subtitle="Derivative of Cauchy Log likelihood (scale=1.)",
56         title="Newton-Raphson")
57 # plotSol(locations, loglikCauchy, newtonMLE,
58 #         xlabel="theta", ylabel="log likelihood",
59 #         subtitle="Cauchy Log likelihood (scale=1.)",
60 #         title="Newton-Raphson",
61 #         zeroLine=FALSE)
62
63 # -----
64 # b. Apply the bisection method with starting points:
65 startPois <- c(-1., 1.)
66 # Use additional runs to illustrate manners in which the bisection method may
67 # fail to find the global maximum.
68
69 # Solve Maximum likelihood Estimation by Bisection Method
70 bisecMLE <- bisection(f=derivLoglikCauchy, a=-1., b=1)
71
72 # -----
73 # c. Apply fixed-point iterations as in (2.29), starting from -1, with scaling
74 # choices of alpha=1, 0.64, and 0.25. Investigate other choices of starting
75 # values and scaling factors.
76
77 # Solve Maximum likelihood Estimation by Fixed Point Method
78 fixedPoiMLE <- fixedPoint(f=derivLoglikCauchy, x0=-1, alpha=0.64)
79
80 # -----
81 # d. From staring values of (theta^(0), theta^(1)) = (-2, -1), apply the secant
82 # method to estimate theta. What happens when (theta^(0), theta^(1)) = (-3, 3),
83 # and for other starting choices?
84
85 # Solve Maximum likelihood Estimation by Fixed Point Method
86 secantMLE <- secant(f=derivLoglikCauchy, x0=-3, x1=3)
87
88 # Plot solutions on their loglikelihood function and its derivative function
89 plotMLE(f=loglikCauchy,
90        newtonMLE, bisecMLE, fixedPoiMLE, secantMLE,
91        xlabel="theta", ylabel="log_likelihood",
92        subtitle="Cauchy_Log_likelihood_(scale=1.)",
93        zeroLine=FALSE)
94 plotMLE(f=derivLoglikCauchy,
95        newtonMLE, bisecMLE, fixedPoiMLE, secantMLE,
96        xlabel="theta", ylabel="derivative_of_log_likelihood",
97
98 subtitle="Derivative_of_Cauchy_Log_likelihood_(scale=1.)",
99 zeroLine=TRUE)
100
101 # -----
102 # e. Use this example to compare the speed and stability of the Newton-Raphson
103 # method, bisection, fixed-point iteration, and the secant method. Do your
104 # conclusions change when you apply the methods to a random sample of size 20
105 # from a N(theta, 1) distribution?
106
107 # Sample data from a N(theta, 1) (theta = 0)
108 data <- rnorm(20, mean=0., sd=1.)
109 # Loglikelihood function of Cauchy distribution (theta, scale=1)
110 loglikNorm <- function(theta, std=1., xs=data) {
111   sum(dnorm(xs, mean=theta, sd=std, log=TRUE))
112 }
113 # Derivative of loglikelihood function of Cauchy distribution (theta, 1)
114 derivLoglikNorm <- function(theta, xs=data) {
115   require(numDeriv)
116   genD(func=loglikNorm, x=theta)$D[1]
117 }
118
119 newtonMLE <- newtonRaphson(f=derivLoglikNorm, x0=mean(data))
120 bisecMLE <- bisection(f=derivLoglikNorm, a=-1., b=0)
121 fixedPoiMLE <- fixedPoint(f=derivLoglikNorm, x0=1, alpha=0.01)
122 secantMLE <- secant(f=derivLoglikNorm, x0=-3, x1=3)
123
124 plotMLE(f=loglikNorm,
125        newtonMLE, bisecMLE, fixedPoiMLE, secantMLE,
126        zeroLine=FALSE)
127
128 plotMLE(f=derivLoglikNorm,
129        newtonMLE, bisecMLE, fixedPoiMLE, secantMLE,
130        ylabel="derivative_of_log_likelihood",
131        subtitle="Derivative_of_Normal_Log_likelihood_(std=1.)",
132        zeroLine=TRUE)
133
134 # Problem 2:
135 # =====
136 # There were 46 crude oil spills of at least 1,000 barrels from tankers in U.S. waters
137 # during 1974-1999. The website for this book contains the following data: the number
138 # of spills in the i-th year, Ni; the estimated amount of oil shipped through US waters
139 # as part of US import/export operations in the i-th year, adjusted for spillage in
140 # international or foreign waters, bi1; and the amount of oil shipped through U.S.
141 # waters during domestic shipments in the i-th year, bi2. The data are adapted from [11].
142 # Oil shipment amounts are measured in billions of barrels (Bbbl).
143
144 # The volume of oil shipped is measure of exposure to spill risk. Suppose we use the
145 # Possion process assumption given by Ni | bi1, bi2 ~ Possion(lambdai) where
146 # lambdai = alpha1 * bi1 + alpha2 * bi2. The parameters of this model are alpha1 and
147 # alpha2, which represent the rate of spill occurrence per Bbbl oil shipped during import/
148 # expert and domestic shipments, respectively.
149 spillsData <- read.table(dataPath, header=TRUE)
150
151 # (Maximize) Objective function
152 loglikPoisson <- function(alpha, data=spillsData) {
153   sum(dpois(data$spills, alpha[1]*data$importexport + alpha[2]*data$domestic, log=TRUE))
154 }
155
156 # -----
157 # a. Derive the Newton-Raphson update for finding the MLEs of alpha1 and alpha2.
158 # b. Derive the Fisher scoring update for finding the MLEs of alpha1 and alpha2.
159 # c. Implement the Newton-Raphson and Fisher scoring methods for this problem,
160 # provide the MLEs, and compare the implementation case and performance of
161 # the two methods.
162 resNewtonMLE <- newtonRaphsonMLE(loglikFunc=loglikPoisson,
163                                theta0=c(3, -1))
164 resFisherMLE <- fisherScoringMLE(loglikFunc=loglikPoisson,
165                                data=spillsData, theta0=c(10, -1))
166
167 plot2DMMLE(loglikPoisson, resNewtonMLE, "Newton_Method")
168 plot2DMMLE(loglikPoisson, resFisherMLE, "Fisher_Scoring")
169
170 # -----
171 # d. Estimate standard errors for the MLEs of alpha1 and alpha2.
172 par(mfrow=c(1, 2))
173 errorAlpha1 <- sqrt((as.vector(resNewtonMLE$iterations[,1]) -
174                        resNewtonMLE$rootApproximation[1])^2)
175 errorAlpha2 <- sqrt((as.vector(resNewtonMLE$iterations[,2]) -
176                        resNewtonMLE$rootApproximation[2])^2)
177
178 plot(errorAlpha1, type="l", xlab="Iteration", ylab="Standard_Error_for_Alpha_1")
179 plot(errorAlpha2, type="l", xlab="Iteration", ylab="Standard_Error_for_Alpha_2")
180
181 # -----
182 # e. Apply the method of steepest ascent. Use step-halving backtracking as
183 # necessary.
184 resAscentBackMLE <- steepestAscentMLE(loglikFunc=loglikPoisson, theta0=c(3, -1),
185                                     alpha0=0.5)
186 resAscentMLE <- steepestAscentMLE(loglikFunc=loglikPoisson, theta0=c(3, -1),
187                                  alpha0=0.05, backtracking=FALSE)
188 plot2DMMLE(loglikPoisson, resAscentBackMLE, "Ascent_Method_with_Backtracking")

```

```

185 plot2DMLE(loglikPoisson, resAscentMLE, "Ascent_Method_without_Backtracking")
186
187 # -----
188 # f. Apply quasi-Newton optimization with the Hessian approximation update given
189 # in (2.49). Compare performance with and without step halving.
190 resQuasiBackMLE <- quasiNewtonMLE(loglikFunc=loglikPoisson, theta0=c(5, -1),
191                                   alpha0=0.2)
192
193 resQuasiMLE <- quasiNewtonMLE(loglikFunc=loglikPoisson, theta0=c(5, -1),
194                               alpha0=0.1, backtracking=FALSE)
195
196 plot2DMLE(loglikPoisson, resQuasiBackMLE, "Quasi_Newton_Method_with_Backtracking")
197
198 plot2DMLE(loglikPoisson, resQuasiMLE, "Quasi_Newton_Method_without_Backtracking")
199
200 # -----
201 # g. Construct a graph resembling Figure 2.8 that compares the paths taken
202 # by methods used in (a)–(f). Choose the plotting region and starting point
203 # to best illustrate the features of the algorithms' performance.

```

## B ROOTFINDER.R APPENDIX

```

1 # Newton Raphson Method
2 newtonRaphson <- function(f, x0, tol=1e-3, n=1000) {
3   # Start the clock!
4   ptm <- proc.time()
5
6   require(numDeriv) # Package for computing f'(x)
7   k <- n # Initialize for iteration results
8
9   # Check the upper and lower bounds to see if approximations result in 0
10  if (f(x0) == 0.) {
11    res <- list("rootApproximation" = x0, "iterations" = c(x0))
12  }
13
14  for (i in 1:n) {
15    dx <- genD(func=f, x=x0)$D[1] # First-order derivative f'(x0)
16    x1 <- x0 - (f(x0) / dx) # Calculate next value x1
17    k[i] <- x1 # Store x1
18    # Once the difference between x0 and x1 becomes sufficiently small,
19    # output the results.
20    if (abs(x1 - x0) < tol) {
21      # Stop the clock
22      dt <- proc.time() - ptm
23      rootApprox <- tail(k, n=1)
24      res <- list("rootApproximation" = rootApprox,
25                "iterations" = k,
26                "time" = dt,
27                "methodName" = "Newton_Raphson")
28      return(res)
29    }
30    # If Newton-Raphson has not yet reached convergence set x1 as x0 and continue
31    x0 <- x1
32  }
33  stop("Exceeded_allowed_number_of_iterations")
34 }
35
36 # Bisection Method
37 bisection <- function(f, a, b, tol=1e-3, n=1000) {
38   # Start the clock!
39   ptm <- proc.time()
40
41   k <- n # Initialize for iteration results
42
43   # If the signs of the function at the evaluated points, a and b,
44   # stop the function and return message.
45   if (!(f(a) < 0) && (f(b) > 0)) {
46     stop('signs_of_f(a)_and_f(b)_differ')
47   }
48   else if (!(f(a) > 0) && (f(b) < 0)) {
49     stop('signs_of_f(a)_and_f(b)_differ')
50   }
51
52   for (i in 1:n) {
53     c <- (a + b) / 2 # Calculate midpoint
54     k[i] <- c
55     # If the function equals 0 at the midpoint or the midpoint is
56     # below the desired tolerance, stop the
57     # function and return the root.
58     if ((f(c) == 0) || ((b - a) / 2) < tol) {
59       # Stop the clock
60       dt <- proc.time() - ptm
61       rootApprox <- tail(k, n=1)
62       res <- list("rootApproximation" = rootApprox,
63                 "iterations" = k,
64                 "time" = dt,
65                 "methodName" = "Bisection")
66       return(res)
67     }
68
69     # If another iteration is required,

```

```

70   # check the signs of the function at the points c and a and reassign
71   # a or b accordingly as the midpoint to be used in the next iteration.
72   ifelse(sign(f(c)) == sign(f(a)),
73          a <- c,
74          b <- c)
75 }
76 # If the max number of iterations is reached and no root has been found,
77 # return message and end function.
78 stop("Exceeded_allowed_number_of_iterations")
79 }
80
81 # Fixed Point Method
82 fixedPoint <- function(f, x0, alpha=1, tol=1e-02, n=1000){
83   # fixed-point algorithm to find x such that x + f(x) == x
84   # assume that fun is a function of a single variable
85   # x0 is the initial guess at the fixed point
86
87   # Start the clock!
88   ptm <- proc.time()
89
90   k <- n # Initialize for iteration results
91
92   if (f(x0) == 0){
93     res <- list("rootApproximation" = x0, "iterations" = c(x0))
94   }
95   for (i in 1:n) {
96     x1 <- x0 + alpha * f(x0)
97     k[i] <- x1
98     if (abs((x1 - x0)) < tol) {
99       # Stop the clock
100      dt <- proc.time() - ptm
101      rootApprox <- tail(k, n=1)
102      res <- list("rootApproximation" = rootApprox,
103                "iterations" = k,
104                "time" = dt,
105                "methodName" = "Fixed_Point")
106      return(res)
107    }
108    x0 <- x1
109  }
110  stop("Exceeded_allowed_number_of_iterations")
111 }
112
113 secant <- function(f, x0, x1, tol=1e-03, n=1000){
114   # Start the clock!
115   ptm <- proc.time()
116
117   k <- n # Initialize for iteration results
118
119   for (i in 1:n) {
120     x2 <- x1 - f(x1) * (x1 - x0) / (f(x1) - f(x0))
121     k[i] <- x2
122     if (abs(f(x2)) < tol) {
123       # Stop the clock
124       dt <- proc.time() - ptm
125       rootApprox <- tail(k, n=1)
126       res <- list("rootApproximation" = rootApprox,
127                 "iterations" = k,
128                 "time" = dt,
129                 "methodName" = "Secant")
130       return(res)
131     }
132     x0 <- x1
133     x1 <- x2
134   }
135   stop("Exceeded_allowed_number_of_iterations")
136 }

```

## C OPTIMIZER.R APPENDIX

```

1 library(MASS)
2
3 newtonRaphsonMLE <- function(loglikFunc, theta0, tol=1e-9, n=1000) {
4   # Start the clock!
5   ptm <- proc.time()
6
7   require(numDeriv) # Package for computing f'(x) and f''(x)
8   k <- matrix(0, ncol=length(theta0)) # Initialize for iteration results
9
10  for (i in 1:n) {
11    deriv <- genD(func=loglikFunc, x=theta0)$D[1:length(theta0)]
12    hess <- hessian(func=loglikFunc, x=theta0)
13    theta1 <- theta0 - deriv %*% solve(hess) # Calculate next value theta1
14    k <- rbind(k, theta1) # Store theta1
15
16    # Once the difference between theta0 and theta1 becomes sufficiently small,
17    # output the results.
18    if (sum(abs(theta1 - theta0)) < tol) {

```



```

19 # Stop the clock
20 dt <- proc.time() - ptm
21 rootApprox <- tail(k, n=1)
22 res <- list("rootApproximation" = rootApprox,
23           "iterations" = tail(k, n=i),
24           "time" = dt,
25           "methodName" = "Newton_Raphson")
26 return(res)
27 }
28 # If Newton-Raphson has not yet reached convergence set theta1 as theta0
29 # and continue
30 theta0 <- theta1
31 }
32 stop("Exceeded_allowed_number_of_iterations")
33 }
34
35 fisherScoringMLE <- function(loglikFunc, data, theta0,
36                             tol=1e-3, n=1000) {
37   # Start the clock!
38   ptm <- proc.time()
39
40   require(numDeriv) # Package for computing f'(x) and f''(x)
41   k <- matrix(0, ncol=length(theta0)) # Initialize for iteration results
42
43   for (i in 1:n) {
44     # Score of loglikelihood
45     score <- genD(func=loglikFunc, x=theta0)$D[1:length(theta0)]
46     # Fisher Information of loglikelihood
47     fisherInfo <- matrix(0, ncol=length(theta0), nrow=length(theta0))
48     for (j in 1:nrow(data)) {
49       estFunc <- function(theta, d=data[j,]) { loglikFunc(theta, d) }
50       estVec <- genD(func=estFunc, x=theta0)$D[1:length(theta0)]
51       fisherInfo <- fisherInfo + estVec%*%t(estVec)
52     }
53     # Update theta by fisher scoring
54     theta1 <- theta0 + MASS::ginv(fisherInfo) %*% score
55     k <- rbind(k, t(theta1)) # Store theta1
56     if (sum(abs(theta1 - theta0)) < tol) {
57       # Stop the clock
58       dt <- proc.time() - ptm
59       rootApprox <- tail(k, n=1)
60       res <- list("rootApproximation" = rootApprox,
61                 "iterations" = tail(k, n=i),
62                 "time" = dt,
63                 "methodName" = "Fisher_Scoring")
64       return(res)
65     }
66     theta0 <- theta1
67   }
68   stop("Exceeded_allowed_number_of_iterations")
69 }
70
71 steepestAscentMLE <- function(loglikFunc, theta0, alpha0=1.,
72                               tol=1e-3, n=1000, backtracking=TRUE) {
73   # Start the clock!
74   ptm <- proc.time()
75
76   require(numDeriv) # Package for computing f'(x) and f''(x)
77   k <- matrix(0, ncol=length(theta0)) # Initialize for iteration results
78
79   alpha <- alpha0
80   for (i in 1:n) {
81     deriv <- genD(func=loglikFunc, x=theta0)$D[1:length(theta0)]
82     # Steepest ascent
83     h <- -1 * alpha * solve(-1 * diag(length(theta0))) %*% deriv
84     # Update theta
85     theta1 <- theta0 + alpha * deriv
86     k <- rbind(k, t(theta1)) # Store theta1
87     # Backtracking by updating alpha
88     if (backtracking && (loglikFunc(theta0) - loglikFunc(theta1) > 0.)) {
89       alpha <- alpha * 0.5
90     }
91     if (sum(abs(theta1 - theta0)) < tol) {
92       # Stop the clock
93       dt <- proc.time() - ptm
94       rootApprox <- tail(k, n=1)
95       res <- list("rootApproximation" = rootApprox,
96                 "iterations" = tail(k, n=i),
97                 "time" = dt,
98                 "methodName" = "Fisher_Scoring")
99       return(res)
100     }
101     theta0 <- theta1
102   }
103   stop("Exceeded_allowed_number_of_iterations")
104 }
105
106 quasiNewtonMLE <- function(loglikFunc, theta0, alpha0=1,
107                             tol=1e-3, n=1000, backtracking=TRUE) {

```

```

108 # Start the clock!
109 ptm <- proc.time()
110
111 k <- matrix(0, ncol=length(theta0)) # Initialize for iteration results
112 # An initial matrix M0 is chosen (usually M0 = I)
113 M <- diag(length(theta0))
114 # An initial alpha alpha0 is chosen
115 alpha <- alpha0
116 for (i in 1:n) {
117   # Update theta
118   deriv0 <- genD(func=loglikFunc, x=theta0)$D[1:length(theta0)]
119   theta1 <- theta0 - alpha * solve(M) %*% deriv0
120   deriv1 <- genD(func=loglikFunc, x=theta1)$D[1:length(theta1)]
121   # Update Matrix M
122   z <- as.vector(theta1 - theta0)
123   y <- deriv1 - deriv0
124   v <- y - M %*% z
125   c <- solve(t(v) %*% z)
126   M <- M + c[1] * (v %*% t(v))
127   # Backtracking by updating alpha
128   if (backtracking && (loglikFunc(theta0) - loglikFunc(theta1) > 0.)) {
129     alpha <- alpha * 0.5
130   }
131   # Update theta
132   k <- rbind(k, t(theta1)) # Store theta1
133   if (sum(abs(theta1 - theta0)) < tol) {
134     # Stop the clock
135     dt <- proc.time() - ptm
136     rootApprox <- tail(k, n=1)
137     res <- list("rootApproximation" = rootApprox,
138               "iterations" = tail(k, n=i),
139               "time" = dt,
140               "methodName" = "Fisher_Scoring")
141     return(res)
142   }
143   theta0 <- theta1
144 }
145 stop("Exceeded_allowed_number_of_iterations")
146 }

```

## D PLOTTER.R APPENDIX

```

1 plotSol <- function(x, yLoglikFunc, resMLE,
2                    xlabel, ylabel, subtitle, title,
3                    zeroLine=TRUE) {
4   # Variables Configurations
5   y <- apply(as.matrix(x), 1, function(v) yLoglikFunc(v))
6   xlters <- resMLE$iterations
7   ylters <- apply(as.matrix(xlters), 1, function(v) yLoglikFunc(v))
8   labellters <- cbind(1:length(xlters), xlters)
9   namebank <- apply(as.matrix(labellters), 1,
10                     function(v) sprintf("iter_%d:_%f", v[1], v[2]))
11   # Plot derivative of loglikelihood function
12   plot(x, y, type="l", xlab=xlabel, ylab=ylabel, sub=subtitle, main=title)
13   if (zeroLine) {
14     abline(h = 0, lty = 2)
15   }
16   points(xlters, ylters, pch=16, col="blue")
17   points(resMLE$rootApproximation, # Root x
18         yLoglikFunc(resMLE$rootApproximation),
19         pch=20, col="red")
20   text(resMLE$rootApproximation, # Root x
21        yLoglikFunc(resMLE$rootApproximation),
22        labels=sprintf("iter_%d:_%f\ntime:_%f", length(xlters), resMLE$rootApproximation, resMLE$tim
23        cex= 0.7, pos=1)
24   }
25
26 plotMLE <- function(f, newtonMLE, bisectionMLE, fixedPoiMLE, secantMLE,
27                    step=1/50, xrange=c(-30, 30),
28                    xlabel="theta", ylabel="log_likelihood",
29                    subtitle="Normal_Log_likelihood_(std=1.)",
30                    zeroLine=TRUE) {
31   par(mfrow=c(2,2))
32   xs <- seq(xrange[1], xrange[2], step) # Range of means to plot
33   plotSol(xs, f, newtonMLE,
34           xlabel=xlabel, ylabel=ylabel, subtitle=subtitle,
35           title=newtonMLE$methodName, zeroLine=zeroLine)
36   plotSol(xs, f, bisectionMLE,
37           xlabel=xlabel, ylabel=ylabel, subtitle=subtitle,
38           title=bisectionMLE$methodName, zeroLine=zeroLine)
39   plotSol(xs, f, fixedPoiMLE,
40           xlabel=xlabel, ylabel=ylabel, subtitle=subtitle,
41           title=fixedPoiMLE$methodName, zeroLine=zeroLine)
42   plotSol(xs, f, secantMLE,
43           xlabel=xlabel, ylabel=ylabel, subtitle=subtitle,
44           title=secantMLE$methodName, zeroLine=zeroLine)
45 }
46

```

```

47 plot2DMLE <- function(f, resMLE, subtitle,
48                       xlim=c(-5, 10), ylim=c(-5, 10), step=1/50) {
49   x <- seq(xlim[1], xlim[2], step)
50   y <- seq(ylim[1], ylim[2], step)
51   u <- as.matrix(expand.grid(x, y)) # Points to evaluate
52   z <- matrix(apply(u, 1, function(v) f(v)), nrow=length(x))
53   contour(x, y, z, nlevels=30, sub=subtitle)
54   # points(resMLE$iterations[,1], resMLE$iterations[,2], pch=16, col="blue")
55   lines(resMLE$iterations[,1], resMLE$iterations[,2],
56         type="o", col="blue")
57   points(resMLE$rootApproximation[1], resMLE$rootApproximation[2],
58         pch=20, col="red")
59   text(resMLE$rootApproximation[1], resMLE$rootApproximation[2],
60        labels=sprintf("iter_%d: %f\ntime: %f",
61                        length(resMLE$iterations[,1]),
62                        resMLE$rootApproximation,
63                        resMLE$time[1]),
64        cex= 0.7, pos=1)
65 }

```