

For this assignment you can do it in a group of maximum three people. Objectives of this assignment:

- To make yourself familiar with R programming (or any other languages).
- To learn about the Newton-Raphson method and its variants.

Altogether there are three questions. You will need to submit your answers (write-up and codes) via canvas.

1. The Cauchy($\theta, 1$) has density

$$p(x - \theta) = \frac{1}{\pi\{1 + (x - \theta)^2\}}.$$

(a) If x_1, \dots, x_n form an i.i.d. sample, show that

$$\begin{aligned} l(\theta) &= -n \log \pi - \sum_{i=1}^n \log\{1 + (\theta - x_i)^2\}, \\ l'(\theta) &= -2 \sum_{i=1}^n \frac{\theta - x_i}{1 + (\theta - x_i)^2}, \\ l''(\theta) &= -2 \sum_{i=1}^n \frac{1 - (\theta - x_i)^2}{\{1 + (\theta - x_i)^2\}^2}. \end{aligned}$$

(b) Show that the Fisher information is $I(\theta) = \frac{n}{2}$.

(c) Use the following data, graph the log likelihood function: $-13.87, -2.53, -2.44, -2.40, -1.75, -1.34, -1.05, -0.23, -0.07, 0.27, 1.77, 2.76, 3.29, 3.47, 3.71, 3.80, 4.24, 4.53, 43.21, 56.75$.

(d) Find the MLE for θ using the Newton-Raphson method (use the same data set as above). Try the following starting points: $-11, -1, 0, 1.4, 4.1, 4.8, 7, 8$, and 38 . Compare your results.

(e) First use Fisher scoring to find the MLE for θ , then refine your estimate using Newton-Raphson. Try the same starting points as above. Compare your results with the previous ones.

2. Consider the following probability density function:

$$p(x) = \frac{1 - \cos(x - \theta)}{2\pi}, \quad 0 \leq x \leq 2\pi,$$

where θ is a parameter between $-\pi$ and π . Use this i.i.d. sample to answer the following questions: $0.52, 1.96, 2.22, 2.28, 2.28, 2.46, 2.50, 2.53, 2.54, 2.99, 3.47, 3.53, 3.70, 3.88, 3.91, 4.04, 4.06, 4.82, 4.85, 5.46$.

(a) Graph the log likelihood function.

(b) Find the method-of-moments estimator for θ . Denote it as $\hat{\theta}_{\text{moment}}$.

(c) Find the MLE for θ using Newton-Raphson with $\theta_0 = \hat{\theta}_{\text{moment}}$.

(d) What solutions do you find when you start at $\theta_0 = -2.7$ and $\theta_0 = 2.7$?

- (e) Repeat the above using 200 equally-spaced starting values between $-\pi$ and π . Partition the values into sets of attraction; i.e., divide the set of starting values into separate groups, with each group corresponds to a unique computed MLE.
3. In chemical kinetics the Michaelis-Menten model is used for modeling the relation between the initial velocity y of an enzymatic reaction and the substrate concentration x . The model is

$$y = \frac{\theta_1 x}{x + \theta_2} + \epsilon, \quad (1)$$

where θ_1 and θ_2 are model parameters and ϵ are iid zero mean normal errors. The following data set is given:

substrate concentration x (ppm)	velocity y [(counts/min)/min]	
0.02	47	76
0.06	97	107
0.11	123	139
0.22	152	159
0.56	191	201
1.10	200	207

We wish to estimate θ_1 and θ_2 by nonlinear least squares; i.e., $\hat{\theta}_1$ and $\hat{\theta}_2$ are defined as the joint minimizer of

$$\sum_{i=1}^n \left(y_i - \frac{\theta_1 x_i}{x_i + \theta_2} \right)^2. \quad (2)$$

- (a) A quick way for finding rough estimates for θ_1 and θ_2 is to invert the relationship in (1) and obtain a simple linear regression setting. That is, ignoring ϵ ,

$$\frac{1}{y} = \frac{x + \theta_2}{\theta_1 x} = \frac{1}{\theta_1} + \frac{\theta_2}{\theta_1} \frac{1}{x} \Rightarrow y^* = \beta_0 + \beta_1 u,$$

where $y^* = 1/y$, $\beta_0 = 1/\theta_1$, $\beta_1 = \theta_2/\theta_1$ and $u = 1/x$. Estimate θ_1 and θ_2 via estimating β_0 and β_1 with least squares.

- (b) Implement a Newton-Raphson algorithm for estimating θ_1 and θ_2 via the minimization of (2). Use your answers from (a) as initial estimates.
- (c) Repeat (b) with the steepest descent algorithm.
- (d) Repeat (b) with the Gauss-Newton algorithm.

—— End of Assignment 1 ——