Stat 580 (Spring 2017): Homework 6

Due, in class, April 20, 2017

Please submit your homework with codes (hard copy) in class and upload the corresponding codes to the Blackboard. Problems marked with * will be graded in detail and they are worth 50% of the total score. Remaining problems, worth the remaining 50% of the total score, will be given full mark if reasonable amount of work is shown.

For this homework, use R for programming parts unless otherwise specified.

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

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

   (a) If $x_1, \ldots, x_n$ 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. 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

$$y = \frac{\theta_1 x}{x+\theta_2} + \epsilon, \tag{1}$$

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

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

(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.