Problem Set 7

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Abstract

This article contains my solutions to Problem Set 7 for the graduate Computational Physics course. Problem Set 7 investigates numerical minimization methods.

1 Problem 1: Brent's Method

Problem 1 involves implementing Brent's 1D minimization method and testing it on the function $y = (x - 0.3)^2 exp(x)$. I implement Brent's method such that its backup method is the Golden section method.

First, I create a function that performs the quadratic interpolation required for Brent's method. Next, I create a function that performs one iteration of the golden section method. This function takes the function in question and the bounds of a bracket as its parameters and returns the new bounds and intermediate point following the iteration of the golden method. The function also returns the size of the step of the iteration, i.e., the size of the change in the bound of the bracket. This step size is needed for when I compare golden section step sizes and interpolation step sizes in Brent's method.

Finally, I implement Brent's method. I start the method with taking a Golden section step to get two endpoints with an intermediate point. Then comes the main method loop. In the loop, I get a new point s from the quadratic interpolation. I then check that s is within the bounds of the current bracket. If it isn't, I simply perform another golden section iteration and proceed to the next iteration of the loop. If s is in the bracket, I then check to see which bracket endpoint is lower on the function. In this step, I will eventually discard whichever bracket endpoint is greater on the function. I then check to see whether s is greater or less than the current bracket midpoint. Depending on where s falls with respect to the current midpoint b, I adjust the bracket endpoints and midpoint with s accordingly and proceed to the next iteration. While this is all happening, I also check to see if the bracket step from the quadratic interpolation is greater than that of the golden section. If it isn't, I will perform a golden section step again and iterate to the next iteration of the loop. If it is, I use the new bracket and midpoint from the interpolation and proceed to the next iteration of the loop. This loop continues until the bracket length is within a certain tolerance, which has a value of 1E-6 in the code I submitted.

My implementation of Brent's method provided that the minimum occurs at 0.29999999, which is very close to the actual value of 0.3. SciPy's Brent method provided a very similar result of 0.3000000002, which makes sense. Both methods provided the correct result.

2 Problem 2: Likelihood Maximization

Problem 2 investigates likelihood maximization for fitting a model the logistic function. In this case, we are investigating whether or not a person's age dictates whether they are familiar with the phrase "Be kind, rewind." The logistic function has the form $p(x) = \frac{1}{1+exp(-(\beta_0+\beta_1 x))}$. We need to maximize the log likelihood of this logistic function with the survey data in order to get the proper beta values for the data.

After reading in the survey data, I create a function for the log likelihood. Then, I need to minimize the negative of this function (maximize the function). In other words, I am maximizing the likelihood function to find the beta values that best fit the logistic function to the survey data. To maximize the likelihood, I create a lambda function that runs the log likelihood function for varying values of beta. I minimize this function using the SciPy optimize minimize method along with the data form the survey. Finally, I use the resultant object from the minimize method to recover the proper values of beta and their errors. I also used the inverse hessian from the result object to find the covariance matrix of the beta values.

The likelihood maximization returned the following values:

$$\beta_0 = -5.62, \beta_1 = 0.11$$

and the following error values:

$$d\beta_0 = 0.004, d\beta_1 = 0.004$$

with a covariance matrix of: $\begin{bmatrix} 1.45E-5 & -1.33E-5 \\ -1.33E-5 & 1.33E-5 \end{bmatrix}$

A plot of the logistic function with the above beta values along with the original survey data is shown in Figure 1. This logistic function does make sense as it follows the trend of the data: increasing probability as age increases. We can see that there is a correlation to a person's age and whether or not they have heard of this phrase before.

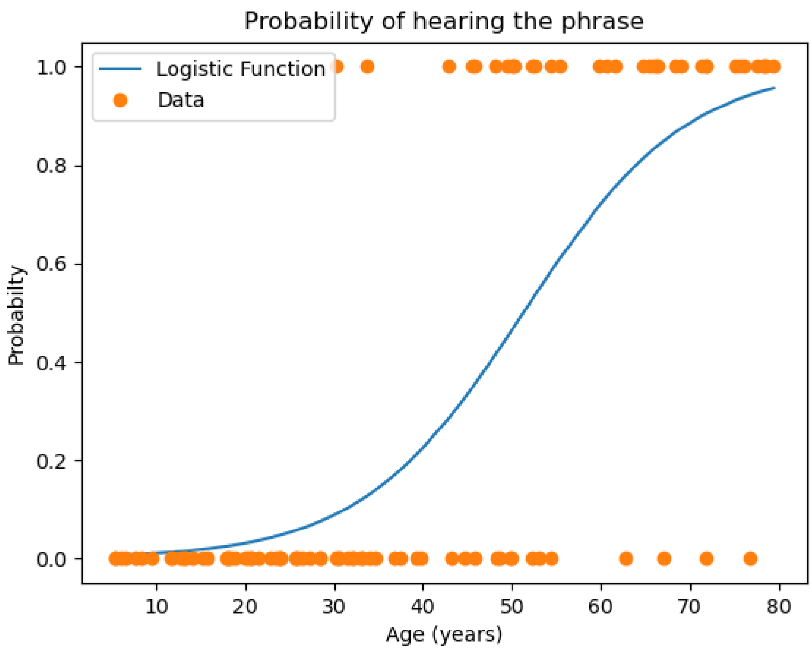

Figure 1: Plot of the calculated logistic function for the survey data. The survey data is also included, with a value of 1 indicating a ”yes” and a value of 0 indicating ”no”.