Science and Computers II: Project 1A

Use of the GNU Scientific Library

This project is intended as an alternative to project 1 for students who are already somewhat familiar with C programming. All material in this project is assessed and your report should document the results of each exercise in a separate section. I suggest writing up the sections as you complete them, rather than leaving all the writing until the end.

The goal of this project is for you to gain familiarity with using a software library to solve a physical problem, rather than writing an entire code from scratch; consequently your programs will likely be quite short. You are not explicitly told which GSL routines to use, as part of the exercise is for you to learn how to locate the appropriate routine to solve a problem.

Before attempting these exercises, you should first read Section 2 of the GSL reference manual

`http://www.gnu.org/software/gsl/manual/html_node/Using-the-library.html`

which explains how to use GSL and link the library into your programs. Then work through the exercises. For each exercise you should identify the relevant numerical problem, e.g. root finding, numerical integration, etc. and then choose an appropriate routine from GSL to solve the problem. If you are having trouble doing this, please see me.

There are four exercises of roughly the same length, so you should to meet the deadline, you should aim to complete one per week.

Exercise 1

The amplitude of the Fraunhoffer diffraction pattern is given by the expression

$$A = A_0 \frac{\sin x}{x}$$

where $x = \frac{1}{2} ka \sin\theta$, k is the wavenumber of the light, a is the slit width and θ is the diffraction angle. Suppose that the wavelength of the light is 589.29 nm and the width of the slit is 2.8 μm. The purpose of this exercise is to find the angles of the maxima in the diffraction pattern. Clearly the values of x for which the zeros occur must satisfy $\sin x = 0$ and therefore are readily determined. What equation must be satisfied by the values of x that correspond to the maxima in the diffraction pattern? The maxima will generally lie between the minima—we therefore have upper and lower bounds for the maxima.

As a general rule: Whenever possible use root-finding routines that bracket the roots—that is safer than using a routine that only asks for an initial approximation.

How many maxima will there be? Call a suitable GSL routine to find the values of x that correspond to these maxima. Finally find the angles corresponding to the maxima. Check your results.

Exercise 2

The error function of mathematical physics is defined by

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp\left(-t^2\right)\, dt$$

Call a suitable GSL routine to evaluate this integral for $-5 < x < 5$ and hence produce a plot of $\mathrm{erf}(x)$ over this range. In fact, there is a GSL routine that returns $\mathrm{erf}(x)$ directly. Call this routine and check that your integral is correct. Call a suitable GSL function to evaluate $\mathrm{erf}(\infty)$ using the above integral. What is its value? How long does it take to calculate the error function of 1,000,000 numbers using your method and the GSL library. Which is faster?

Hint: The Unix `time` command can be used to measure the time that a process takes to run.

Exercise 3

Integrate the following simple differential equations over the specified ranges of x. Find the solutions numerically and check your results against an analytic calculation.

$$\frac{\mathrm{d}y}{\mathrm{d}x} = y, \quad y(0) = 1, \quad 0 < x < 2$$

$$\frac{\mathrm{d}^2y}{\mathrm{d}x^2} = -4y, \quad y'(0) = 1, \quad y(0) = 10, \quad 0 < x < 4\pi$$

Exercise 4

Consider the following 3×3 matrix:

$$\begin{pmatrix} 1 & 2 & 3 \\ 2 & 2 & 3 \\ 3 & 3 & 3 \end{pmatrix}$$

Using suitable GSL functions find (a) its inverse, (b) its determinant, (c) its eigenvalues and eigenvectors.

Write a program that generates matrices of size 1000×1000, 2000×2000, ..., up to $10,000 \times 10,000$. How long does it take the computer to find the determinant of such a matrix? You must be careful not to print the matrices out to `stderr` or `stdout`, or this will slow the calculation. How does the timing scale with the problem? How long do you think it would take to find the determinant of a $10^6 \times 10^6$ matrix?