3rd Year B.Sc. Honours Examination 2012 B6

Programming and Scientific Computation - PH306

9.00 am- 12.00 pm. April 19, 2013

Instructions: Answer the following questions. The mark for each part of a question is indicated on the right. Once done writing and executing codes, **please copy them in the exam book**. Any plot that you make, **must be saved for later viewing**.

Time: 3 hours. **Total Marks**: 25

1. The Laguerre polynomials $L_n(x)$ has the series representation:

$$L_n(x) = \sum_{k=0}^{n} \frac{(-1)^k n! x^k}{(n-k)!k!k!}$$

where $n = 0, 1, 2, 3, \ldots$ are integers.

   (a) Write a `C` or `C++` function `double laguerren(double x, int n)` that evaluates the Laguerre polynomials $L_n(x)$ using the above definition. You will need to define your own factorial function for this. [4+2]

   (b) In a complete `C` or `C++` program write the values of x in the first column and the values of the function $L_n(x)$ in consecutive columns for $n = 0, 1, 2, 3, 4$. Plot, using `gnuplot` the functions $L_n(x)$ in the range $x \in [0, 5]$ using the above C/C++ function for different $n = 0, 1, 2, 3, 4$ in the same plot. Save the plot as a postscript file. [2+2]

2. The Laplace's method for evaluating integrals of the type $\int_a^b \exp\left(Mf(x)\right)\, \mathrm{d}x$, where $f(x)$ is an at least twice-differentiable function with a global maximum, and M is a large number is given by:

$$\int_a^b \exp\left(Mf(x)\right)\, \mathrm{d}x \approx \exp\left(Mf(x_0)\right)\sqrt{\frac{2\pi}{M|f''(x_0)|}}$$

where at x_0, the function $f(x)$ has a global maximum and hence $f'(x_0) = 0$.

   (a) Define a function $f(x)$ in `C` or `C++` as `double f(double x)` which is given by [2]

$$f(x) = \frac{\sin x}{x} = \begin{cases} 1 & \text{if } x = 0 \\ \sin(x)/x & \text{if } x \neq 0 \end{cases}$$

   (b) Using any suitable numerical integration scheme, write a `C` or `C++` function `double numlpc(double M)` that evaluates the above integral $\int_a^b \exp\left(Mf(x)\right)\, \mathrm{d}x$ for a given value of the positive parameter M, between the limits $a = -10, b = 10$. You will need the above definition of the function `double f(double x)`. [5]

   (c) Write another function `double aprlpc(double M)` that evaluates the above approximate value of the integral for the positive parameter M. Use $f(x_0) = 1$, $f''(x_0) = -1/3$. [2]

   (d) Call the above two functions `numlpc(M)` and `aprlpc(M)` in a complete `C` or `C++` program and write the values of x in the first column and the function values `numlpc(M)` and `aprlpc(M)` in consecutive columns in a file. Plot `numlpc(M)` and `aprlpc(M)` versus x using `gnuplot` in a single plot and save the plot as a postscript file. [3]

3. (a) Use the series representation of Laguerre polynomials $L_n(x)$ given by:

$$L_n(x) = \sum_{k=0}^{n} \frac{(-1)^k n! x^k}{(n-k)!k!k!}$$

   where $n = 0, 1, 2, 3, \ldots$ are integers, to define a `Maple` functions `mylague(n,x)` to evaluate the Laguerre polynomials of orders $n = 0, 1, 2, \ldots 4$. [1]
   [Hint: The `Maple` symbol for factorial of n is $n!$].

   (b) Using `Maple`, plot $L_n(x)$ for $n = 0, 1, 2, \ldots 5$ in the same plot for $x \in [0, 4]$. [1]

   (c) Using `Maple` evaluate the first three derivatives of the Laguerre polynomials i.e. $L_n'(x)$, $L_n''(x)$ and $L_n^{(3)}(x)$ for $n = 4$. [1]

Save the worksheet that contains the `Maple` commands that you wrote and the plot.

$$csch(x) = \frac{1}{x} + 2x \sum_{k=1}^{\infty} \frac{(-1)^k}{x^2 + (k\pi)^2}$$

for $x \neq 0$

(a) Define a C or C++ function `double cosech(double x, int n)` that evaluates the series expansion for the Fresnel integral using the expansion up to the n-th term in the series for a given value of the arguments x and n. [5]

(b) Plot your function `cosech(x,n)` with $n = 20$, for $x \in [0.1, 1.0]$ using `gnuplot` and save the plot as a postscript file. [2+1]

2. The Legendre Polynomials have the integral representation

$$P_n(x) = \frac{1}{\pi} \int_0^{\pi} \left[x + \sqrt{x^2 - 1} \cos\phi\right]^n \mathrm{d}\phi$$

(a) Write a `Maple` procedure or function, `legendre(n,x)`, that evaluates the Legendre Polynomial of order n, using the above relations, at some point x. [3]

(b) Using `Maple`, evaluate

$$\int_{-1}^{1} P_m(x) P_n(x) \mathrm{d}x$$

for $m \neq n$ and $m = n$. Take $m, n = 1, 2, 3, \ldots$ etc. [2]

(c) Using `Maple`, plot $P_3(x)$ and $P_5(x)$. [2]

(d) Using `Maple`, find the zeros of $P_3(x)$. [1]

1. The Euler's method for solving the second order ordinary differential equation $\mathrm{d}^2x/\mathrm{d}t^2 + \omega^2 x = 0$, written as a set of coupled first order difference equations is

$$\begin{aligned} x_{n+1} &= x_n + f(x_n, t_n)(t_{n+1} - t_n) = x_n + z_n h \\ z_{n+1} &= z_n + g(z_n, x_n, t_n)h = z_n - \omega^2 x_n h \end{aligned}$$

Consider the initial conditions $x_0 = 0$, $z_0 = 1$.

(a) Write a C/C++ code that solves the above initial value problem. Your code should write the values of t, x and z in different columns of a file. [6]

(b) Plot the values of $z = \frac{\mathrm{d}x}{\mathrm{d}t}$ vs. x for $\omega = 1, 4, 9, 16$. [3]

2. The electron and the nuclear charge densities of the hydrogen atom are given by

$$\rho_e(r) = -\frac{q}{\pi} e^{-2r}, \qquad \rho_p(r) = q\delta(\vec{r})$$

where we have adopted the system of units in which the Bohr radius $a_0 = 1$ and $k_e = 1/(4\pi\epsilon_0) = 1$. The system is spherically symmetric and hence volume integration of a radial function $f(r)$ can be expressed as $\int f(r)\mathrm{d}^3r = 4\pi \int_{r=0}^{\infty} f(r)\, r^2 \mathrm{d}r$. Also, recall that $\int \delta(\vec{r})\mathrm{d}^3r = 1$
Hint: The `Maple` function for the Dirac delta function $\delta(r)$, is `Dirac(r)`. Use `Pi` for π in `Maple` instead of `pi`.

(a) Using `Maple` find the total positive and negative charges of the atom. Do your answers make sense? [2]

(b) Using `Maple` evaluate

$$\int_{-\infty}^{\infty} j_m(x) j_n(x) \mathrm{d}x, \qquad m,\, n \geq 0$$

for (a) $m \neq n$ and (b) $m = n$ taking $m, n = 0, 1, 2, \ldots$ etc. Can you interpret the result? Can you guess the value of the integral for general m, n? [2+0.5+0.5]

3. (a) Using `Maple`, evaluate the magnetic field at a distance D for in infinitely long wire procedure `laguerre:=proc(n,x)`, that recursively calculates the Laguerre Polynomial of order n, using the above relations, at some point x. [5]

(b) Use the above procedure `laguerre(n,x)` to calculate the values of $n!L_n(x)$ for $n = 1, 2, \ldots 4$ and plot them. [2]