3rd Year B.Sc. Honours Examination 2012 B9

Programming and Scientific Computation - PH306

2.00 pm- 5.00 pm. April 20, 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 Bernoulli Polynomials have fourier series representations

$$\begin{aligned} B_{2n}(x) &= (-1)^{n+1}\frac{2(2n)!}{(2\pi)^{2n}}\sum_{k=1}^{\infty}\frac{\cos(2\pi kx)}{k^{2n}}, \qquad \text{even order} \\ B_{2n+1}(x) &= (-1)^{n+1}\frac{2(2n+1)!}{(2\pi)^{2n+1}}\sum_{k=1}^{\infty}\frac{\sin(2\pi kx)}{k^{2n+1}}, \qquad \text{odd order} \end{aligned}$$

   (a) Write a `C` or `C++` function `double bernpoly(double x, int s, int M)` that evaluates the Bernoulli polynomials of order s using the above Fourier series representations using the first M terms in the infinite series. Take suitable value of M for evaluating the function $\mathrm{B}_s(x)$. [Hint: For $s = 2n$, use $n = s/2$, and for $s = 2n + 1$, use $n = (s - 1)/2$.] [6]

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

2. The semi-empirical mass formula for nuclear binding energy is given by:

$$B = aA - bA^{2/3} - s\frac{(A-2Z)^2}{A} - \frac{dZ^2}{A^{1/3}} - \frac{\delta}{A^{1/2}}$$

   where $a = 15.835$ (MeV), $b = 18.33$ (MeV), $s = 23.20$ (MeV), $d = 0.714$ (MeV), $\delta = 0$ for even-odd nuclei, $+11.2$ (MeV) for odd-odd nuclei and -11.2 (MeV) for eevn-even nuclei.

   (a) Write a `C` or `C++` function `double getA(double B, int Z)` that will give the mass number A given the binding energy B and the atomic number Z. Use any suitable root-finding method. [6]

   (b) Use the above function in a complete `C` or `C++` program to estimate the mass numbers of deuteron and tritium given their binding energies as $B = 2.224589$ (MeV) and $B = 8.481821$ (MeV), respectively. [2+1+1]

3. An integral representation for the Weber function $\mathrm{E}_n(x)$ is are given by:

$$\mathrm{E}_n(x) = \frac{1}{\pi}\int_0^{\pi}\sin(nt - x\sin(t))\mathrm{d}t$$

   (a) Write a `Maple` functions `E(n,x)` that evaluates the Weber function $\mathrm{E}_n(x)$ using the above definition, at some point x. [Hint: The `Maple` symbol for π is `Pi`]. [1]

   (b) Using `Maple`, plot $\mathrm{E}_n(x)$ for $n = 0.0, 0.5, 1.0, 1.5, 2.0$ in the same plot for $x \in [-8, 8]$. [2]

   (c) Using `Maple` evaluate the first, second and third derivatives of the Weber function i.e. $\mathrm{E}_n^{'}(x)$, $\mathrm{E}_n^{''}(x)$ and $\mathrm{E}_n^{(3)}(x)$ for $n = 0, 1$. [0.5+0.5]

   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]