3rd Year B.Sc. Honours Examination 2012 B10

Programming and Scientific Computation - PH306

9.00 am- 12.00 pm. April 21, 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. Random numbers may be used to calculate integrals. This method is known as Monte Carlo Integration. Consider the Fresnel integrals $C(z)$ and $S(z)$:

$$C(z) = \int_0^z \cos\frac{\pi x^2}{2} \mathrm{d}x, \qquad \text{and} \qquad S(z) = \int_0^z \sin\frac{\pi x^2}{2} \mathrm{d}x$$

   (a) Generate a sequence of pair of random numbers (x, y) with $x \in [0, z]$ and $y \in [0, 1]$. Write `C` or `C++` functions `double C(double z, int N)` and `double C(double z, int N)` to calculate the value of the Fresnel integrals by comparing the areas under the curves $y = \cos(\pi x^2)/2$ and $y = \sin(\pi x^2)/2$ with that of the rectangular region with sides z and 1 using N pairs of random numbers, i.e. N points. [5]

   (b) Increase the number of points used to evaluate the area and find the errors in each case. Take $N \in [10, 10^7]$. The exact value of the integrals for $z = 1$ are $C(1) = 0.77989340037682282947\ldots$ and $S(1) = 0.43825914739035476608\ldots$, respectively. [2]

   (c) Write the number of points and the errors in two consecutive columns of a file. Plot the errors vs the number of points used and the save the plot as a postscript file. [2+1]

2. The Dawson integrals appear in physics in various fields including spectroscopy, heat conduction, electrical conduction, propagation of electromagnetic radiation along the earth's surface, etc. The Dawson integrals are defined as

$$\begin{aligned} D_+(x) = F(x) &= \exp(-x^2) \int_0^x \exp(t^2) \, \mathrm{d}t \\ D_-(x) &= \exp(x^2) \int_0^x \exp(-t^2) \, \mathrm{d}t \end{aligned}$$

   (a) Write two `C` or `C++` functions `double dawpos(double x)` and `double dawmin(double x)` that returns the Dawson integrals $D_+(x)$ and $D_-(x)$, respectively, at some points x, using any suitable numerical integration scheme. Take suitable number of grid points. [6]

   (b) In a complete `C` or `C++` program write the values of x in the first column and the values of the functions $D_+(x)$ in the second and $D_-(x)$ in third column. Plot, using `gnuplot` the functions $D_+(x)$ in the range $x \in [-6, 6]$ and $D_-(x)$ in the range $x \in [-2, 2]$ using the above C/C++ functions. Save the plots as postscript files. [2+2]

3. The Bernoulli Polynomials have fourier series representations

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

   (a) Write `Maple` function `Be(s,x)` and `Bo(s,x)` that evaluate Bernoulli polynomials of even and odd orders $B_{2n}(x)$ and $B_{2n+1}(x)$, respectively using the above definition, at some point x. [Hint: The `Maple` symbol for π is `Pi` and the factorial of n is represented as $n!$. For $s = 2n$, use $n = s/2$, and for $s = 2n + 1$, use $n = (s - 1)/2$.]. [1+1]

   (b) Using `Maple`, plot `Be(s,x)` or `Bo(s,x)`, as appropriate, for $s = 1, 2, 3, 4, 5$, in the same plot for $x \in [-8, 8]$. [2]

   (c) Using `Maple` evaluate the first, second and third derivatives of the Bernoulli polynomials i.e. $B_s^{'}(x)$, $B_s^{''}(x)$ and $B_s^{(3)}(x)$ for $n = 3, 4$. [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]