3rd Year B.Sc. Honours Examination 2012 B4

Programming and Scientific Computation - PH306

2.00 pm- 5.00 pm. April 04, 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 following integral

$$I = \int_{-\pi}^{\pi} \frac{\exp(-x^2)}{1+\cos^2(x)} \mathrm{d}x$$

   (a) Generate a sequence of pair of random numbers (x, y) with $x \in [-\pi, \pi]$ and $y \in [0, 0.5]$. Write a `C` or `C++` function `double integral2(int N)` to calculate the value of the integral by comparing the area under the curve $y = \exp(-x^2)/(1+\cos^2(x))$ and that of the rectangular region with sides 2π and 0.5 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 integral is $1.0964423232264471296\ldots$. [2]

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

2. In celestial mechanics, Kepler's Equation relates the mean anomaly M to the eccentric anomaly E of an elliptical orbit of eccentricity e as:

$$M = E - e\sin(E)$$

   The orbital eccentricities (e) of the first six planets in the solar system are 0.2056, 0.0068, 0.0167, 0.0934, 0.0483, 0.0560; the mean eccentricity of the Moon's orbit is 0.0549.

   (a) Write a `C` or `C++` function `double eccanom(double M, double e)` that will calculate the eccentric anomalies E for a planet or the Moon for given values of M and e using any suitable root finding method. [4]

   (b) Call `eccanom(M,e)` in a complete `C` or `C++` program and write the values of E in different columns of a file for each planet and the Moon when the mean anomaly $M \in [\pi/4, \pi/2]$ radians and varying M in steps of $\Pi/80$. Plot the values in a single plot using `gnuplot` and save the plot as a postscript file. [3+2]

   (c) Are there values for the eccentric anomaly for which $E = M$? If so, what are they? [1+1]

3. An integral representation for the Hermite polynomials $H_n(x)$ is given by:

$$H_n(x) = \frac{2^{n+1}}{\sqrt{\pi}} \exp(x^2) \int_0^{\infty} \exp(-t^2) t^n \cos(2xt - n\pi/2) \mathrm{d}t$$

   (a) Write a `Maple` function `Hermi2(n,x)`, that evaluates the Hermite polynomials $H_n(x)$, using the above definition, at some point x. [2]
   [Hint: The `Maple` symbol for $i = \sqrt{-1}$ is `I` and that for π is `Pi`].

   (b) Using `Maple`, plot $H_n(x)$ for $n = 1, 2, 3, 4$ in the same plot for $x \in [0, 2]$. [2]

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

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

(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]