3rd Year B.Sc. Honours Examination 2011B7

Programming and Scientific Computation - PH306

10.00 am- 1.00 pm. May 12, 2012

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. A continued fraction representation for the function $\tan^{-1}(x)$ (as a sequence of fractions) is given by

$$c_0 = x, \quad c_1 = \frac{x}{1+(1x)^2}, \quad c_2 = \frac{x}{1+\dfrac{(1x)^2}{3+(2x)^2}}, c_3 = \frac{x}{1+\dfrac{(1x)^2}{3+\dfrac{(2x)^2}{5+(3x)^2}}}, \ldots \tan^{-1}(x) = \frac{x}{1+\dfrac{(1x)^2}{3+\dfrac{(2x)^2}{5+\dfrac{(3x)^2}{7+\dfrac{(4x)^2}{9+\cdots}}}}}$$

   (a) Write a C or C++ function `double myarctan(double x,int n)`, that evaluates the n-th order iterated value of $\tan^{-1}(x)$ using the above algorithm. [4]

   (b) Call the function `double myarctan(double x, int n)` in a complete C or C++ program and evaluate $\tan^{-1}(x)$ with $n \in [0, 20]$ and write the values in a data file. [2]

   (c) Plot the values of $|\text{myarctan}(x, n) - \tan^{-1}(x)|$ at $x = 1.0$, versus n in the range $[0, 20]$ using `gnuplot`. Save your plot as a postscript file. [2]

2. For a square-well potential given by

$$V(r) = \begin{cases} -V_0 & \text{for} \quad r < R \\ 0 & \text{for} \quad r > R \end{cases}$$

the energy eigenvalues $|E| = V_0(1-\xi^2)$, lying in the range $0 < E < V_0 \Rightarrow 0 < \xi < 1$, are given by the equation:

$$\tan(x_0\xi) = f_l(x_0, \xi)$$

where $l = 0, 1, 2, \ldots$ is the angular momentum quantum number and the functions $f_l(x_0, \xi)$ for $l = 0, 1$ are given by

$$f_0(x_0, \xi) = -\frac{\xi}{\sqrt{1-\xi^2}}, \qquad f_1(x_0, \xi) = \frac{x_0\xi}{1 + \left(\xi^2/(1-\xi^2)\right)\left(1 + x_0\sqrt{1-\xi^2}\right)}$$

   (a) Plot the three functions $\tan(x_0\xi)$, $f_0(x_0, \xi)$ and $f_1(x_0, \xi)$, in the same plot for $x_0 = 10$ and in the range $0 < \xi < 1$ and save it as a postscript file.Besides the trivial case for $\xi = 0$, there should be three points of intersection, between the two graphs of $\tan(x_0\xi)$ and $f_l(x_0, \xi)$ for both $l = 0, 1$. Take $x_0^2 = 2mV_0R^2/\hbar^2 = 100$. [3]

   (b) Write a C or C++ program to find all the six possible energy states taking $V_0 = 1$ using any suitable root finding algorithm. [6]
   [Hint:A few roots of the equation $\tan(x_0\xi) = f_l(x_0, \xi)$ are near $\xi = 0.28, 0.56, 0.84$ for $l = 0$.]

3. The Planck's distribution law is given by

$$R_T(\nu) = \frac{2\pi h}{c^2} \frac{\nu^3}{\exp(h\nu/kT) - 1}$$

   (a) Define a `Maple` expression `R` that is equal to $R_T(\nu)$ as given above. You do not need to write a function of ν [1]

   (b) Using `Maple`, evaluate $R_{\text{int}}(\nu) = \int_0^\infty R_T(\nu)\text{d}\nu$ assuming $c > 0$, $h > 0$, $k > 0$ and $T > 0$. Use `Maple` command `assuming` to take positive values of h, c, k, T. [2]

   (c) Using `Maple`, evaluate $\sigma = R_{\text{int}}(\nu)/T^4$. [1]

   (d) Using `Maple`, find the value of frequency ν, at a particular temperature T and in terms of k and h, at which $R_T(\nu)$ becomes maximum. You may want to use differentiation and `Maple` command `solve` to find it. [2]

   (e) Using `Maple` plot $R_T(\nu)$ at $T = 1000, 1500, 2000$ K with the values of $c = 2.9979e8$, $k = 1.38e-23$, $h = 6.626e-34$ in the same plot. Put legends for each plot and take the range $\nu \in [0, 4.0e14]$. [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. A continued fraction representation for the Golden Ratio ϕ is given by (as a sequence)

$$x_1 = 1 + \frac{1}{1}, \quad x_2 = 1 + \cfrac{1}{1+\cfrac{1}{1}}, \quad x_3 = 1 + \cfrac{1}{1+\cfrac{1}{1+\cfrac{1}{1}}}, \quad \ldots\ldots \quad \phi = 1 + \cfrac{1}{1+\cfrac{1}{1+\cfrac{1}{1+\cfrac{1}{1+\cdots}}}}$$

The sequence $\{x_n\}$ converges to $\phi = 1.6180339887498948482045868343656\ldots$ as the number of iterations goes to infinity.

(a) Write a C or C++ function `double mygold(int n)`, that evaluates the n-th order iterated value of ϕ i.e. x_n, using the above algorithm. [4]

(b) The Golden Ratio may be used to compute the Fibonacci numbers using the relation below:

$$f_n = \frac{1}{2\phi - 1}\left(\phi^{n+1} - (1-\phi)^{n+1}\right), \qquad \text{for} \quad n = 2, 3, \ldots$$

This is an amazing equation. The right-hand side involves powers and quotients of irrational numbers, but the result is a sequence of integers.

Write a C or C++ function `double myfibo(n)` that evaluates the n-th order Fibonacci number using the above algorithm and approximating to the nearest integer value. [4]

(c) Call `double myfibo(n)` in a complete C or C++ program and output Fibonacci numbers for $n \in [1, 11]$. For you comparison, the corresponding Fibonacci numbers are: { 1,2,3,5,8,13,21,34,55, 89, 144 }. [2]

2. The generating function for the Hermite polynomials $H_n(x)$ is $g(x,t) = \exp(-t^2 + 2tx)$, such that

$$\sum_{n=0}^{\infty} \frac{H_n(x)}{n!} t^n = g(x,t) = \exp(-t^2 + 2tx)$$

(a) Use the `taylor` command to generate the first five Hermite polynomials from the above definition of the generating function. [2]

(b) Use the `coeftayl` command to write a `Maple` function, `hermite(n,x)`, that evaluates the Hermite function of order n, using the above relation, at some point x. [2]

(c) Using `Maple`, plot $H_n(x)$ for $n = 1, 2, 3, 4$ in the range $x \in [-5, 5]$ in a single plot. [1]

(d) Using the above `Maple` function `hermite(n,x)`, evaluate: [1]

$$\int_{-\infty}^{\infty} H_m(x)H_n(x)e^{-x^2}\mathrm{d}x$$

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

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]

4. 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 $\int \delta(\vec{r})\mathrm{d}^3 r = 1$
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]

5. (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]