3rd Year B.Sc. Honours Examination 2011B5

Programming and Scientific Computation - PH306

10.00 am- 1.00 pm. May 10, 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 $\tan(x)$ (as a sequence of fractions) is given by

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

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

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

   (c) Plot the values of $|\mathrm{mytan}(x, n) - \tan(x)|$ at $x = \pi/4$, versus n in the range $[0, 20]$ using `gnuplot`. Save your plot as a postscript file. [2]

2. The electrostatic potential at a point (x, y) on the $xy-$plane due to a uniform surface charge distribution ρ in the square region $-1 \le x' \le 1$, $-1 \le y' \le 1$ is given by

$$V(x, y) = \frac{\rho}{4\pi\epsilon_0}\int_{-1}^{1}\int_{-1}^{1}\frac{1}{\sqrt{(x-x')^2+(y-y')^2}}\mathrm{d}x'\mathrm{d}y'$$

   (a) Write a C or C++ program that evaluates the electrostatic potential at the point (x, y) using any suitable numerical integration technique. Take $\rho/(4\pi\epsilon_0) = 1$ [5]

   (b) Save data from your program for $V(y, x)$ at the three values of $y = 1.5, 2.0, 2.5$ in the range $x \in (1.5, 10)$. Plot the data using `gnuplot` and save the plot as a postscript file. [2+1]

3. The Bose-Einstein integral function is defined as

$$g(\sigma, z) = \frac{1}{\Gamma(\sigma)}\int_0^{\infty}\frac{x^{\sigma-1}}{e^x z^{-1} - 1}\mathrm{d}x$$

   (a) Define a `Maple` function `g(sigma,z)` that evaluates the above function. Plot `g(sigma,z)` for $z \in [0, 1]$ with $\sigma = 1, 1, 5, 3$ in the same plot. [1+1]

   (b) Using `Maple` command `taylor`, expand the function `g(sigma,z)` around $z = 0$ assuming $\sigma > 0$. You may want to use the `Maple` command `assume` to take consider positive values of σ. [1]

   (c) Using `Maple` command `convert`, convert the Taylor series expansion above into a polynomial and define a `Maple` function `h1(sigma,z)` that is equal to the polynomial. [2]

   (d) Using `Maple` command `subs`, express the above function `h1(sigma,z)` in terms of the new variable $\alpha = -\ln(z)$ and define a `Maple` function `h2(sigma,alpha)` that is equal to `h1(sigma,z)`. [2]

   (e) The Mellin transformation of a function $f(\alpha)$ is defined as

$$Z(s) = \int_0^{\infty} f(\alpha)\alpha^{s-1}\,\mathrm{d}\alpha$$

   Using `Maple`, evaluate the Mellin transform of $h2(\sigma, \alpha)$. [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 $\phi = 1.6180339887498948482045868343656...$ 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]