3rd Year B.Sc. Honours Examination 2011B3

Programming and Scientific Computation - PH306

10.00 am- 1.00 pm. May 09, 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. The period of a simple pendulum for large angle amplitude (θ_M) may be written as

$$T = 2\pi\sqrt{\frac{L}{g}}\frac{1}{M\left(\sqrt{1-\sin^2\frac{1}{2}\theta_M}\right)}$$

where $0 \le \theta_M < \pi$ and $M(x)$ is the **arithmetic-multiplicative mean**, defined as

$$M(x) = \lim_{n\to\infty} a_n, \qquad \text{where} \qquad a_1 = x, b_1 = 1, \quad a_{n+1} = \frac{a_n + b_n}{2}, \; b_{n+1} = \sqrt{a_n b_n}$$

   (a) Write a C or C++ function `double artmul(double x, int n)`, that evaluates the n-th order iterated value of the above sequence that approximates the arithmetic-multiplicative mean $M(x)$ at x. [3]

   (b) Write a C or C++ function `double pendulumT(double thetaM)`, that evaluates the period T for a given θ_M as the argument using the above definition and the function `double artmul(double x, int n)`. Choose the value of L/g such that, as $\theta_M \to 0$, $T = 1\,\text{s}$ and take a large value of n. Call the function `pendulumT()` from the `main()` function with different values of θ_M as input. [4]

   (c) Using the above function, plot T vs. θ_M for $\theta_M \in [0, \pi/2]$. [2]
   Hint: Check values: $\theta_M = [10°, 50°, 90°] \Rightarrow T = [1.00193, 1.05033, 1.18258]$.

2. In theory of probability, the gamma distribution function is given by

$$f(x;\alpha,\beta) = \frac{1}{\beta^\alpha\Gamma(\alpha)}x^{\alpha-1}\exp\left(-x/\beta\right) \qquad x > 0; \quad \alpha, \beta > 0$$

where $\Gamma(\alpha) = (\alpha-1)!$, for integer α, is the gamma function.

   (a) Write a C or C++ function `double gammadist(double x, int alpha, double beta)` that evaluates the beta distribution function using the above definition and the factorial function. [2]

   (b) Write a C or C++ program that evaluates the gamma distribution function for different values of α and $\beta = 2$.
   Using the function `double gammadist(x,alpha,beta)`, evaluate (ii) $\langle x\rangle$ i.e. the mean value of x and (ii) $\sigma^2 = \langle x^2\rangle - \langle x\rangle^2$, i.e. the variance of x, using different $\alpha = 1, 2, 3, 4, \ldots$ and $\beta = 2$. Take the range of x as $[0, X]$, where X is a sufficiently large number. You may use any numerical integration method of your choice. [4]

   (c) Plot (ii) $\langle x\rangle$ and (ii) σ^2 with respect to α using `gnuplot` and save the plots in a postscript file. [1.5+1.5]

3. The gamma function is defined by the infinite product representation as

$$\Gamma(z) = \lim_{n\to\infty}\frac{1}{z}\prod_{i=1}^{n}\left(1+\frac{z}{i}\right)^{-1} n^z$$

   (a) Define a `Maple` function `mygamma(z)` that uses the above definition. [3]

   (b) Using `Maple`, plot `mygamma(x)` and `|mygamma(x)|` for $x \in [-5, 5]$ between the values $y \in [-5, 5]$. [1+1]

   (c) Evaluate `mygamma(1/2 -n) mygamma(1/2+n)` for different n=1,2,3,.... Can you guess the general result? [1+1]

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 $g(x,t) = \exp\left(-t^2 + 2tx\right)$, such that

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

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

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]