3rd Year B.Sc. Honours Examination 2011$_{\text{B1}}$

Programming and Scientific Computation - PH306

10.00 am- 1.00 pm. May 08, 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 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 $\phi = 1.61803398874989484820458683436 56...$ 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. In theory of probability, the beta distribution function is given by

$$f(x;p,q) = \frac{1}{B(p,q)} x^{p-1}(1-x)^{q-1} \qquad 0 \le x \le 1; \quad p, q > 0$$

where $B(p,q) = \int_0^1 t^{p-1}(1-t)^{q-1}\mathrm{d}t$, is the beta function.

   (a) Write a C or C++ function `double betadist(double x, double p, double q)` that evaluates the beta distribution function using the above two definitions. You may use any numerical integration method of your choice. [5]

   (b) Write a C or C++ program that evaluates the beta distribution function for different values of p, q and $x \in [0,1]$. Take (p,q) equal to $(2,2)$ and $(3,3)$. Plot $f(x;p,q)$ with respect to x for $x \in [0,1]$ using `gnuplot` and save the plots in a postscript file. [2+2]

3. 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 .

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

(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]