Assignment – UECM3033 Numerical Methods

(Jan 2013)

Objectives:

1. To train students to carry out work/assignment responsibly.
2. To train students such that they could communicate and work together with other people effectively.
3. To consolidate students knowledge in numerical methods and its applications.

Introduction

This assignment consists of two parts, which consist of two mini projects. Part A is application of root finding algorithm and numerical integration. Part B is a problem related to initial value problem.

This assignment will be carried out individually. At the end of the assignment, every student will need to submit a report (not more than 4 pages) on the mini projects.

In the assignment, the work must be the work of the individuals, and help received from others, and sources of information (e.g. books or articles) must be properly acknowledged. Plagiarism is an serious offend, student found to be guilty of plagiarism will be liable to disciplinary actions.

Deadline

Finally, **the deadline of the assignment is 5.00 pm 21 March 2013 (Thursday of Week 10).** Reports submitted after the deadline will **NOT** be marked, unless an extension has been granted by the lecturer.

Do not wait until last minute to work on this assignment.

Mini Project A: Numerical Integration, and Roots Finding [Total: 10 marks]

Choose one of the following functions to carry out the assignment:

- $f(x) = \int_{0.1}^{x} e^{-t^2}\, dt$, where $0.1 < x < 5$
- $f(x) = \int_{0.1}^{x} \sin(t)/t\, dt$, where $0.1 < x < 5$
- $f(x) = \int_{0.1}^{x} e^{-t} \cos(t)\, dt$, where $0.1 < x < 5$

1. Write a python/matlab program and name it `nInt.py` or `nInt.m`.
    - The program `nInt` will return the value of $f(x)$ when input a numerical value of x, where $0.1 < x < 5$.
    - The program `nInt` will use a composite Simpson's rule to calculate $f(x)$ with 1000 equally spaced partitions.
2. Show that there is at least one interception point for $f(x)$ and $y = 1 - x/5$ in the interval $0.1 < x < 5$.
3. Find the interception point with either:
    - secant method; or
    - Newton's method.
4. Plot $f(x)$, $y = 1 - x/5$ and the interception point on a same graph.
5. Comment on the accuracy of the interception point estimation, and how you will be able to improve the estimation.

Mini Project B: Numerical Differential Equations [Total: 10 marks]

Consider a particle in two dimensions with Cartesian coordinates x and y, and momentum (p_x, p_y). The state of the system can be represented as a point (x, y, p_x, p_y) in four-dimensional phase space. Suppose the particle has potential energy $V(x, y)$ and mass 1. Then, its total energy is

$$H = \frac{1}{2}(p_x^2 + p_y^2) + V(x, y), \tag{1}$$

and the equations of motion can be written as (Hamiltons equations)

$$\frac{dx}{dt} = \frac{\partial H}{\partial p_x} = p_x, \tag{2}$$

$$\frac{dy}{dt} = \frac{\partial H}{\partial p_y} = p_y, \tag{3}$$

$$\frac{dp_x}{dt} = -\frac{\partial H}{\partial x} = -\frac{\partial V}{\partial x}, \tag{4}$$

$$\frac{dp_y}{dt} = -\frac{\partial H}{\partial y} = -\frac{\partial V}{\partial y}. \tag{5}$$

The solution to this system of equations, for given initial values $(x(0), y(0), p_x(0), p_y(0))$, can be represented as a curve in phase space, $t \mapsto (x(t), y(t), p_x(t), p_y(t))$. Along this curve the energy is conserved. Hence, the curve falls on a three-dimensional hypersurface S_E corresponding to constant H,

$$S_E = \{(x, y, p_x, p_y) : H(x, y, p_x, p_y) = E = \text{constant}\}.$$

The following are some of the common potentials that used in modelling physical problems:

Hénon-Heiles Potential	$V = \frac{1}{2}\left(x^2 + y^2\right) + x^2 y - \frac{1}{3}y^3$
Central Potential	$V = \left(x^2 + y^2\right)^2$

Choose one of the above potential and answer the following questions:

1. Plot the equipotential curves for the potential. The equipotential curve is represented by the curve $\{(x, y) : V(x, y) = \text{constant}\}$, where along this curve the potential V is constant.
   - For the Hénon-Heiles potential, plot the equipotential curves for $V = 1/6, 0.1, 0.05$, and 0.01.
   - For the Central potential, plot the equipotential curves for $V = 1/6, 0.1, 0.05$, and 0.01.
2. Write three programmes to solve the Hamilton equations numerically using the following three methods:
   (a) Euler method (you are required to write your own code)
   (b) Runge-Kutta 45 method (you are encouraged to use the built-in function from matlab/python.)
   (c) Predictor-corrector method (you are required to write your own code)

   Use an initial condition of $x = y = p_y = 0$ and p_x is calculated from the initial energy E; step size $h = 0.001$ and iterate until time $T = 100$.
3. In your assignment report, please include the following: In your programme, you have to
   - plot the curves of $p_x(t)$ versus $x(t)$, and $p_y(t)$ versus $y(t)$ on a same graph. Use an energy parameter, E, of your own choice and $E < 0.1$. Comment the graph.
   - plot the curves for E versus t for the three different methods on a same graph and comment.

——————ooOO The End & Good Luck OOoo——————