DEPARTMENT OF PHYSICS
INDIAN INSTITUTE OF TECHNOLOGY, MADRAS

PH5720 Numerical Methods and Programming **Session 08** **17 March 2020**
Time: 2:00 pm - 5:00 pm **[Total: 10 points]**

Goal of this session:

1. Root finding algorithms.
2. Beginners (only Problem 1, 2, 3 and 4), Advanced: (full sheet)
3. You may use the codes uploaded on moodle for examples/syntax etc.
4. Please submit this lab sheet, upload all your codes and data files on moodle by **Tuesday 31 March 2020, 5:00 pm**.

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1. Multiple-Choice Test

   (a) Assuming an initial bracket of [1,5], the second (at the end of 2 iterations) iterative value of the root of $te^{-t} - 0.3 = 0$ using the bisection method is

      i. 0
      ii. 1.5
      iii. 2
      iv. 3

   (b) For an equation like $x^2 = 0$, a root exists at $x = 0$. The bisection method cannot be adopted to solve this equation in spite of the root existing at $x = 0$ because the function $f(x) = x^2$

      i. is a polynomial
      ii. has repeated roots at $x = 0$
      iii. is always non-negative
      iv. has a slope equal to zero at $x = 0$

   (c) The false-position method may have difficulty in finding the root of $f(x) = x^2 - 7.4x + 13.69 = 0$ because

      i. $f(x)$ is a quadratic polynomial
      ii. $f'(x)$ is a straight line
      iii. one cannot find initial guesses x_L and x_U that satisfy $f(x_L)f(x_U) < 0$
      iv. the equation has two identical roots.

   (d) The root of the equation $f(x) = 0$ is found by using the Newton-Raphson method. The initial estimate of the root is $x_0 = 3$, $f(3) = 5$. The angle the line tangent to the function $f(x)$ makes at $x = 3$ is $57°$ with respect to the x-axis. The next estimate of the root, x_1 most nearly is

i. - 3.2470
ii. - 0.2470
iii. 3.2470
iv. 6.2470

(e) The ideal gas law is given by $pv = RT$ where p is the pressure, v is the specific volume, R is the universal gas constant, and T is the absolute temperature. This equation is only accurate for a limited range of pressure and temperature. Vander Waals came up with an equation that was accurate for larger ranges of pressure and temperature given by $\left(p+\frac{a}{v^2}\right)(v-b) = RT$ where a and b are empirical constants dependent on a particular gas. Given the value of $R = 0.08$, $a = 3.592$, $b = 0.04267$, $p = 10$ and $T = 300$ (assume all units are consistent), one is going to find the specific volume, v, for the above values. Without finding the solution from the Vander Waals equation, what would be a good initial guess for v ?

i. 0
ii. 1.2
iii. 2.4
iv. 3.6

2. Write a code which implements the bisection method, Newton-Raphson's method and secant method. Find the positive roots of

$$x^2 - 4xsinx + (2sinx)^2 = 0,$$

using these three methods and compare the achieved accuracy number of iterations needed to find the solution. Give a critical discussion of the methods provided the space below.

3. Make thereafter a C++ class which includes the above three methods and test this class against selected problems of your own.

4. Root finding: Find the roots of

$$f(x) = x^2 - R$$

for $R = 13$ using the following root finding methods:

(a) Bisection

(b) Newton-Raphson Method

Comment on the convergence of the algorithms below:

5. A Physics Problem: In this problem, we will obtain the binding energy of a deuteron, which is a bound state of a neutron and a proton. If we switch to the relative frame, we can cast this two-body problem into an equivalent one-body problem. The radial part of the Schrödinger equation is

$$-\frac{\hbar^2}{m}\frac{d^2u(r)}{dr^2} + V(r)u(r) = Eu(r) \tag{1}$$

where $u(r)$ is the radial part of the wave function, E is the energy eigenvalue, m is the reduced mass defined as

$$m = 2\frac{m_n m_p}{m_n + m_p} \tag{2}$$

m_n, m_p are the masses of the neutron and the proton respectively. Let us assume that they are nearly equal. If we consider the following potential

$$V(r) = -V_0 \qquad 0 \leq r < a \tag{3}$$

$$V(r) = 0 \qquad \text{otherwise} \tag{4}$$

then we can solve the radial equation in two regions $0 \leq r < a$ and $r \geq a$. We then match the wave function and its derivative at $r = a$. It is easy to show that we end up with a transcendental equation:

$$k\cot(ka) = -\beta \tag{5}$$

where

$$k = \sqrt{m(V_0 - |E|)}/\hbar, \tag{6}$$

and

$$\beta = \sqrt{m|E|}/\hbar. \tag{7}$$

Use $V_0 = 60\text{MeV}$, $a = 1.45\text{fm}$ and $m = 938\text{MeV}/c^2$ and $\hbar c = 200\text{MeV fm}$ plot the function in Eq. 5 by first defining

$$f(E) = k\cot(ka) + \beta \tag{8}$$

(a) Look for a solution i.e. $f(E) = 0$ graphically. This plot helps you narrow in on the initial guesses for the root finders. What is the root you get graphically?

(b) Find the eigenvalue E using the different root finding techniques (Bisection, Newton-Raphson and Secant). Compare the number of iterations for a predetermined accuracy.

6. (Bonus) In the above problem, what is the critical value of V_0 (critical depth) below which you can have a bound state?