EM 314 - Assignment 2: SOLUTIONS

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November 26, 2018

1. Consider the bisection algorithm to solve an equation $f(x) = 0$, starting with an interval $[a, b]$. Show that the minimum number of iterations k required to achieve a tolerance τ satisfy

$$k > \log_2 \left(\frac{b-a}{\tau} \right) - 1,$$

Hint: Refer the error estimate of the bisection method.

Solution: From the error estimate we have

$$e_k = |x_k - x_*| \leq \frac{b-a}{2^{k+1}}$$

We need $e_k < \tau$. Thus,

$$\begin{aligned} \frac{b-a}{2^{k+1}} &< \tau \\ \frac{b-a}{\tau} &< 2^{k+1} \\ \log_2 \left(\frac{b-a}{\tau} \right) &< k+1 \end{aligned}$$

and the result follows.

2. Consider the function $g(x) = e^{-x}$.

(a) Prove that g is a contraction on $G = [\ln 1.1, \ln 3]$.

Solution: $g'(x) = -e^{-x} \leq 0 \quad \forall x$. Hence, $g(x)$ is a monotonically decreasing function. Now,

$$|g'(x)| = e^{-x} \leq e^{-\ln 1.1} = \frac{1}{1.1} < 1.$$

Thus, g is a contraction on G.

(b) Prove that $g : G \to G$.

Solution: $G = [\ln 1.1, \ln 3] = [0.0953, 1.0986]$. We have proved that $g(x)$ is a continuous monotonically decreasing function. Also,

$$g(\ln 1.1) = e^{-\ln 1.1} = 1/1.1 = 0.9091,$$
$$g(\ln 3) = e^{-\ln 3} = 1/3 = 0.3333.$$

Thus, $g : G \to [g(\ln 3), g(\ln 1.1)] \subset G$.

(c) Deduce that $x_{k+1} = g(x_k)$ converges to the unique fixed point $x_* \in G$ for **any** $x_0 \in G$.

Solution: Follows immediately from (a), (b) and the Banach Fixed Point Theorem.

3. (a) Consider the fixed point iteration $x_{k+1} = g(x_k)$ where $g(x) = \tan^{-1}(2x)$. Clearly, $x = 0$ is a fixed point of $g(x)$. Show that fixed point iteration will not converge to this fixed point.

Solution: For any $x_0 \neq 0$, $x_k \neq 0\ \forall k$. Thus, to achieve convergence with a tolerance $\tau \leq 1/2$, we need $x_k \in [-1/2, 1/2]$ for some k. Hence, it suffices to consider the interval $[-1/2, 1/2]$. Now,

$$g'(x) = \frac{2}{1+4x^2}.$$

From MVT,

$$|x_{k+1} - 0| = |g(x_k) - g(0)| = |g'(\xi)||x_k - 0|, \quad 0 < |\xi| < |x|.$$

Thus, for all $x_k \in [-1/2, 1/2]$, we have $|g'(x)| > 1$ resulting $|x_{k+1}| > |x_k|$. Therefore $x_k \nrightarrow 0$ and the fixed point iteration will not converge to $x_* = 0$.
Note: I omitted the "Hint" I have given in the assignment.

(b) There is another fixed point x_* near $x = 1.16$.

(i) Starting with an initial guess $x_0 = 2$, write 2 iterations of the fixed point iteration method to find x_*. At each iteration k, clearly indicate the approximate solution x_k and the error estimate e_k.

(ii) Redo part (i) using the Newton's method.

Solution: Let $x_0 = 2$.
Fixed point iteration: $x_{k+1} = \tan^{-1}(2x_k)$

$$\begin{aligned} x_1 &= 1.32582 \quad e_1 = |x_1 - x_0| = 0.11565 \\ x_2 &= 1.21016 \quad e_2 = |x_2 - x_1| = 0.03117 \end{aligned}$$

Now, x_* is a solution of $f(x) \equiv \tan^{-1}(2x) - x = 0$.

$$f'(x) = \frac{2}{1+4x^2} - 1 = \frac{1-4x^2}{1+4x^2}.$$

Thus, the Newton's method:

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)} = x_k - \frac{[\tan^{-1}(2x_k) - x_k](1+4x_k^2)}{1-4x_k^2}$$

$$\begin{aligned} x_1 &= 1.23593 \quad e_1 = |x_1 - x_0| = 0.76407 \\ x_2 &= 1.16697 \quad e_2 = |x_2 - x_1| = 0.06895 \end{aligned}$$

4. Implementation of Newton's Method + some experiments.

Solution: Discussed in the lab class.

5. **Kepler's Equation.**
The Cartesian coordinates of a planet in an elliptic orbit at time t are equal to $(ea \sin E, \cos E)$, where a is the semimajor axis, and e is the eccentricity of the ellipse. Using Kepler's laws of planetary motion, it can be shown that the angle E, called the eccentric anomaly, satisfies Kepler's Equation:

$$M = E - e \sin E, \quad 0 < |e| < 1,$$

where M is called the mean anomaly.

Suppose $e = 0.8$, $M = 3$. Solve Kepler's Equation using Newton's method. Use your code in Question 4 with $\tau = 10^{-8}$.

Solution: Let $f(x) = x - e \sin x - M$ with $e = 0.8, M = 3$.
Also, $f'(x) = 1 - e \cos x$. Solving $f(x) = 0$ using Newton's method, we obtain the eccentric anomaly, $E = 3.06289 \quad (rad)$.

6. **State Equation of a Gas**
The Van der Waals equation of state for a gas is given by

$$\left\{ p + a \left(\frac{N}{V} \right)^2 \right\} (V - Nb) = kNT,$$

where V is the volume occupied by the gas, T is the temperature, p is the pressure, N is the number of molecules contained and k is the Boltzmann constant. a and b are coefficients that depend on the specific gas.

Use bisection method to find the volume occupied by 1000 molecules of CO_2 at a temperature $T = 300K$ and a pressure $p = 3.5 \times 10^7 Pa$, with a tolerance of 10^{-12}. For carbon dioxide (CO_2) $a = 0.401 Pam^6, b = 42.7 \times 10^{-6} m^3$. The Boltzmann constant is $k = 1.3806503 \times 10^{-23} JK^{-1}$.

Solution: Let

$$f(V) = pV^3 - (Nbp + kNT)V^2 + (aN^2)V - abN^3$$

We can implement this function in Octave as follows:

```
function y = f(x)

p=3.5*(10^7);
a=0.401;
N=1000;
```

```
b=42.7*10^(-6);
k=1.3806503*(10^(-23));
T=300;

y = p*(x.^3) + a*(N^2)*x - a*b*(N^3) -(N*b*p+k*N*T)*x.^2;
```

We use bisection method to solve $f(V) = 0$. (Use bisection.m.)

```
 >> [zero, res, niter] = bisection(@f,0,1,10^(-12),100)

zero =
    0.0427

res =
  -1.4883e-08

niter =
    38
```

Thus, the volume $= 0.0427m^3$.