# NE451 Solution: Homework assignment 1

**Fall 2019. Instructor: Dr. Jeff Chen**

**Prob. 1.** [2-3. Computational] Write a program to implement Lagrange's interpolating method. On entrance to the program, $t_0, t_1, ...t_n$ and $x_0, x_1, ..., x_n$ are used as input through a data file. Another input parameter is $n$ which can be used to control the dimension of the vector as well as the degree of the interpolating polynomial. This should be input through a data file as well, or automatically identified after the initial data set for $t_i$ and $x_i$ is imported. Interactively, the user will be asked to input the value of $t$. The approximation based on the polynomial interpolation, $p$, is then calculated and printed on screen. A warning message would be printed if $t$ is outside the region $[t_0, t_n]$ of the known data points.

**Solution** The following components are expected:

[code] Attach your code (but will not be marked).

[Example of description of your code] The program sets up arrays $T(n+1)$ and $X(n+1)$ and then opens a file called "Ini.dat", which contains

$n$
$t0\ x0$
...
$tn\ xn$

The first loop reads these data into the program. The user is then asked to input $t$ through an on screen query: "Input your t". Read $t$ and determine if it is within $[t_0, t_n]$. If not, print an error message. If yes, perform two loops in $i$ and $j$.

Start loop $i$ from 0 to $n$.

Loop-$j$: Going through $j = 0$ to $j = n$ but $j \neq i$. Obtain the product

$$P_i = \prod_{j \neq i} \left( \frac{t - t_j}{t_i - t_j} \right).$$

End loop-$j$.

Sum up...

$$p = p + x_i P_i$$

End loop-$i$.

Return to user query for repeated input.

[Test] The Initial file is

5
0 3
0.2 6
0.4 10
0.6 15
0.8 20

Running the program we have:

"Input your t?"
0.35
"p=" *** (your answer)
"Input your t?"
2
"Outside the t range" (error message).

**Prob. 2.** [2-3, Analytical]Show that the function $\Psi_n(x)$

$$\Psi_n(t) = (t - t_0)(t - t_1)...(t - t_n) \qquad (1)$$

has the following properties. For $n = 1$, Max $|\Psi_1(x)| = \alpha_1 h^2$ and for $n = 2$, Max $|\Psi_2(x)| = \alpha_2 h^3$, where $h$ is the uniform step size used in dividing $x$ and $\alpha_1$ and $\alpha_2$ are two numerical constants. What are the values of $\alpha_1$ and $\alpha_2$?

**Solution**

$[n = 1]$

We have

$$\Psi_1(t) = (t - t_0)(t - t_1).$$

From $d\Psi/dt = (t - t_1) + (t - t_0) = 0$, we obtain

$$t_{\max} = (t_0 + t_1)/2$$

Substituting it back to $\Psi$ we have

$$\Psi_1(t_{\max}) = (h/2)^2$$

Hance

$$\alpha_1 = 1/4.$$

$[n = 2]$

We have

$$\Psi_2(t) = (t - t_0)(t - t_1)(t - t_2).$$

Letting $t_0 = -h$, $t_1 = 0$ and $t_2 = h$ for easier calculation. From $d\Psi/dt = t(t - h) + (t + h)(t - h) + (t + h)t = 0$, we obtain

$$3t^2 - h^2 = 0.$$

Hence

$$t_{\max} = \pm \frac{h}{\sqrt{3}}.$$

$$\Psi_{\max} = (h^2/3 - h^2)\frac{h}{\sqrt{3}} = \frac{2}{3\sqrt{3}} h^3$$

$$\alpha_2 = \frac{2}{3\sqrt{3}}.$$

**Prob. 3.** [2-7, Analytical] Consider three data points, $(t_{-1}, x_{-1})$, $(t_0, x_0)$ and $(t_1, x_1)$, where $t_1 - t_0 = t_0 - t_{-1} = h$.
(a) Write down a quadratic polynomial to represent the interpolated function.
(b) Take the derivative of the interpolation polynomial at $t_0$ to represent the derivative of the interpolated function. Discuss the results. Estimate the error of the approximation to the "original" derivative in terms of magnitude of $h$ on the basis of considering the error represented by Weierstrass' Theorem.
(c) Take the second derivative of the interpolation polynomial at $t_0$ to represent the second derivative of the interpolated function. Estimate the error of the approximation to the "original" derivative in terms of magnitude of $h$ on the basis of considering the error represented by Weierstrass' Theorem.

**Solution**

(a)

$$p_2(t) = \frac{1}{h^2}\left[\frac{x_1}{2}t(t+h) + \frac{x_{-1}}{2}t(t-h) - x_0(t^2-h^2)\right]$$

(b) Taking derivative...

$$dp_2(t)/dt = \frac{1}{h^2}\left[\frac{x_1}{2}(2t+h) + \frac{x_{-1}}{2}(2t-h) - x_0(2t)\right].$$

Letting $t = 0$

$$dp_2(t)/dt = (x_1 - x_{-1})/2h.$$

[Discussion] It is the central difference formula for the first derivative.
[Estimate error] Weierstrass:

$$E(t) = \frac{1}{6}(t+h)t(t-h)x^{(3)}[\zeta(t)].$$

Taking derivative we have

$$E'(t) = \frac{1}{6}(3t^2 - h^2)x^{(3)}[\zeta(t)] + \Psi_2(t)x^{(4)}\zeta'(t).$$

Letting $t = 0$ leads to

$$E'(0) = \frac{-h^2}{6}x^{(3)}[\zeta(t)] = \mathcal{O}(h^2)$$

(c) Taking second derivative...

$$d^2p_2(t)/dt^2 = \frac{1}{h^2}\left[x_1 + x_{-1} - 2x_0\right].$$

[Discussion] It is the central difference formula for the second derivative.
[Estimate error] Weierstrass: From the above, we have

$$E'(t) = \frac{1}{6}(3t^2 - h^2)x^{(3)}[\zeta(t)] + \Psi_2(t)x^{(4)}\zeta'(t).$$

Therefore,

$$E''(t) = \frac{1}{6}(6t)x^{(3)}[\zeta(t)] + \Psi_2'(t)x^{(4)}\zeta'(t) + \Psi_2(t)\frac{d[x^{(4)}\zeta'(t)]}{dt}$$

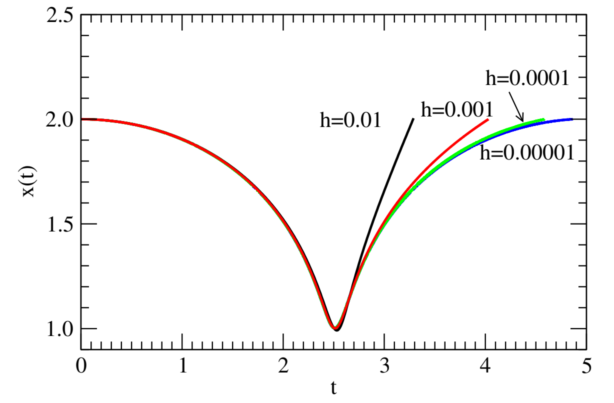


FIG. 1: Trajectory $x(t)$ within $t = [0, T]$. The black, red, green and blue curves are produced by letting $h = 10^{-2}, h = 10^{-3}, h = 10^{-4}$ and $h = 10^{-5}$. Euler's method is used.

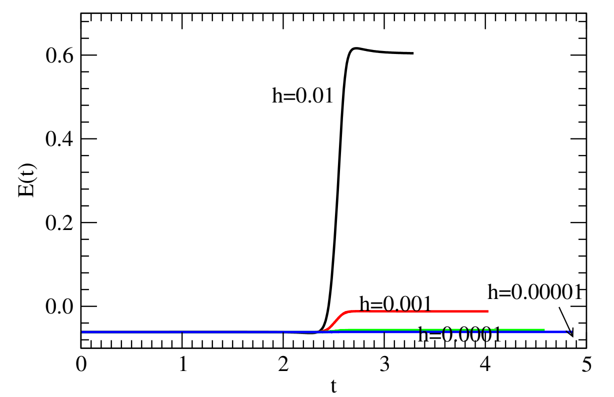


FIG. 2: Total energy $E(t)$ within $t = [0, T]$. The black, red, green and blue curves are produced by letting $h = 10^{-2}, h = 10^{-3}, h = 10^{-4}$ and $h = 10^{-5}$. Euler's method is used.

where

$$\Psi_2' = 3t^2 - h^2.$$

Letting $t = 0$ we have

$$E''(0) = 0 + \Psi_2'(0)x^{(4)}\zeta'(t) + 0 = \mathcal{O}(h^2)$$

**Prob. 4.** [2-9, Euler, Computational] A one-dimensional particle is moving in the force field $F(x) = (48/x^{13} - 24/x^7)$ where $x$ is the distance from the origin. The initial conditions are $x(0) = 2$ and $v(0) = 0$. The particle will first accelerate towards the origin because of the attraction and then decelerated because of the repulsion. Calculate the trajectory $x(t)$ for the time duration $[0, T]$, where $T$ is the approximate time when the particle reaches $x = 2$ again, after reversing its direction of motion.
(a) Use Euler's method to solve Newton's equation of motion, by adopting $h = 10^{-2}, 10^{-3}, 10^{-4}$, $h = 10^{-5}$, etc. Plot $x(t)$ for (at least) 4 cases on one graph.

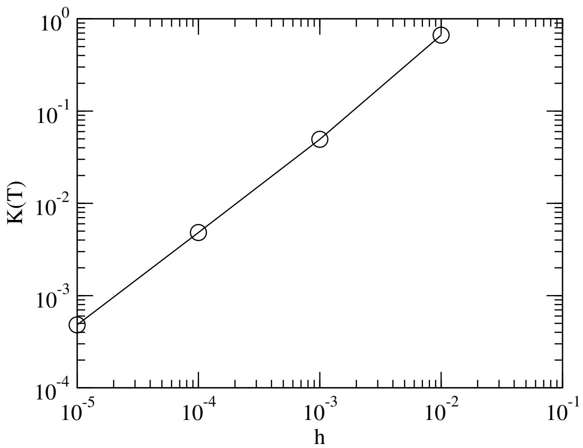


FIG. 3: Kinetic energy at time $t = T$. Euler's method is used.

(b) Compute the total energy $E(t)$ as a function of $t$ and plot on the same graph for selected $h$.
(c) Consider your kinetic energy at $T$, $K(T) = (1/2)v^2$. According to conservation of energy, $K_{\mathrm{exact}}(T) = 0$. Plot your computed $K(T)$ as a function of $h$ in logarithmic-logarithmic scales. Discuss your findings.

**Solution**

[Code] Attach your code

[Example of description of your code] On entrance, the program reads $h$, $x_0$ and $v_0$,from a file named "Ini.dat". Initialization:

$$t = 0$$

Then, a loop in $t$ is constructed such that

$$t = t + h.$$

The following two quantities are calculated,

$$x_1 = x_0 + hv_0$$

$$v_1 = v_0 + hf(x_0),$$

where $f(x_0)$ is the force,

$$f(x_0) = (48/x_0^{13} - 24/x_0^7).$$

IF $(x_0 > 2)$, then $T = t$, do your analysis, end your program. Otherwise, $x_0 = x_1$ and $v_0 = v_1$. Calculate Etot... (how? Explain your steps). Write to a file, $t, x(t), E(t)$. go back to loop-t; ENDIF.

Here is the analysis part.

$$K = v_0^2/2$$

Write to a file, $h$ and $K$.

[Final results]

(a) Trajectories for the selected $h$. See Fig. 1.

(b) $E(t)$ for the selected $h$. See Fig. 2.

(c) $K(T)$ as a function of $h$. See Fig. 3.