ASSIGNMENT-5

→ Sangram Keshari Patro

Q2) (programme is attached)

For 3-point.

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{6} f'''(\xi) \longrightarrow (1)$$

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - \frac{h^2}{12} f^{(4)}(\xi) \longrightarrow (2)$$

For - 5-point

$$f'(x) = \frac{f(x-2h) - 8f(x-h) + 8f(x+h) - f(x+2h)}{12h} + \frac{h^4}{30} f^{(5)}(\xi) \rightarrow (3)$$

$$f''(x) = \frac{-f(x-2h) + 16f(x-h) - 30f(x) + 16f(x+h) - f(x+2h)}{12h^2} + \frac{h^4}{90} f^{(6)}(\xi) \rightarrow (4)$$

for 3-point $\boxed{(e^x) \text{ at } x=0}$ $\boxed{1^{st} \text{ derivate}}$

Exact value = 1 but using 24-bit arithmetic I got the results, we can see that if h decrease then error decreses but after some h it starts increasing.

from → (1) for h_{opti}

$$\frac{2\epsilon}{2h} = \frac{h^2}{6} M_3 \Rightarrow h_{opt} = \left(\frac{6\epsilon}{M_3}\right)^{1/3} = \left(\frac{6\hbar M_0}{M_3}\right)^{1/3} \rightarrow (5)$$

$(\epsilon = \hbar M_0)$

so $h_{opt} \simeq (6\hbar)^{1/3} \simeq 0.007$

and the corresponding error bound $= \frac{2\epsilon}{h_{opt}} = \frac{2\hbar M_0}{\left(6\hbar \frac{M_0}{M_3}\right)^{1/3}} \simeq \left(\frac{4\hbar^2}{3}\right)^{1/3} \simeq 2\times10^{-5} \longrightarrow (6)$

And from the program we can see, at 0.005 the error is 5×10^{-6} which is reasonably close to the theoretical value which is calculated.

for 5-point (for h_{opt}.)

from -eq-(3) → $\frac{18\epsilon}{12h} = \frac{h^4}{30} M_5 \Rightarrow h_{opt} = \left(\frac{45\hbar M_0}{M_5}\right)^{1/5} \simeq (45\hbar)^{1/5} \simeq 0.08 \rightarrow (7)$

and the error bound $= \frac{3\epsilon}{h_{opt}} = \frac{3\hbar M_0}{\left(\frac{45\hbar M_0}{M_5}\right)^{1/5}} \simeq \left(\frac{27\hbar^4}{5}\right)^{1/5} \simeq 2\times10^{-6} \longrightarrow (8)$

and from the program we can see at 0.01 (closer to 0.08) the error is 3×10^{-6} which is again close to the theoretical value which is calculated.

$\boxed{\text{2nd derivative}}$ e^x at $x=0$

· for 3-point
exact value = 1.

From eq-(2) → for h optimum

$$\frac{4\epsilon}{h^2} = \frac{h^2}{12}M_4 \Rightarrow h_{opt} = \left(\frac{48\hbar M_0}{M_4}\right)^{1/4} \simeq (48\hbar)^{1/4} \simeq 0.04 \quad (9)$$

and the error bound $= \frac{8\epsilon}{h_{opt}^2} = \frac{8\hbar M_0}{\left(\frac{48\hbar M_0}{M_4}\right)^{1/2}} \simeq \left(\frac{4\hbar}{3}\right)^{1/2} \simeq 3\times10^{-4}$ (10)

From the program we can see, at $h = 0.05$ (closer to 0.04) the error is 2×10^{-4} which is resonably close to the theoretical value calculated.

for 5-point

from → eq → (4) for h optimum (11)

$$\frac{\cancel{64}\,16\,\epsilon}{\cancel{12}\,3\,h^2} = \frac{h^4}{90}M_6 \Rightarrow h_{opt} = \left(\frac{480\hbar M_0}{M_6}\right)^{1/6} \simeq (480\hbar)^{1/6} \simeq 0.2$$

and the total error bound $= \frac{32\epsilon}{3h_{opt}^2} = \frac{32\hbar M_0}{3\left(\frac{480\hbar M_0}{M_6}\right)^{1/3}} \simeq \left(\frac{1024\hbar^2}{405}\right)^{1/3}$ (12) $\simeq 2\times10^{-5}$

from the ~~program~~ program we can see at $h = 0.1$ (closer to 0.2) the error is 1×10^{-5} which is resonably close to the theoretical value calculated

Now for tan x at $h = ~~1~~\,1.56$
Correct value ÷ $f'(x) = 8579.556$
$f''(x) = 1589286$

From the program we can observe that the error start decreasing with h & reaches some optimum value & again start increasing. (At $\frac{\pi}{2}$ the function blows)

1st derivative for 3-point.

$$h_{opt} = \left(\frac{6\hbar M_0}{M_3}\right)^{1/3} \simeq 4\times10^{-5}$$

$$\text{error} = \frac{2\hbar M_0}{\left(\frac{6\hbar M_0}{M_3}\right)^{1/3}} \simeq 4\times10^{-5}$$

★ [using $|f^{(k)}(x)| \doteq \frac{k!}{\left(\frac{\pi}{2}-x\right)^{k+1}}$
$\frac{\pi}{2} \simeq 1.57$ so $\frac{\pi}{2} - 1.56 \simeq 0.01$
for $k = 1, 2 \ldots 6$]

1^{st} derivative for 5-point

$$h_{opt} = \left(\frac{45\hbar M_0}{M_5}\right)^{1/5} \simeq 3\times10^{-4} \text{ \& error} = \frac{3\hbar M_0}{\left(\frac{45\hbar M_0}{M_5}\right)^{1/5}} \simeq 7\times10^{-6}$$

2^{nd} derivative for - 3 point

$$h_{opt} = \left(\frac{48\hbar M_0}{M_4}\right)^{1/4} \simeq 2\times10^{-4} \text{ \& error} = \frac{8\hbar M_0}{\left(\frac{48\hbar M_0}{M_4}\right)^{1/2}} \simeq 9\times10^{-4}$$

2^{nd} derivative for 5-point

$$h_{opt} = \left(\frac{480\hbar M_0}{M_6}\right)^{1/6} \simeq 6\times10^{-4} \text{ \& error} = \frac{32\hbar M_0}{3\left(\frac{480\hbar M_0}{M_6}\right)^{1/3}} \simeq 10^{-4}$$

we can ~~see~~ observe from the program that these values are reasonably close to the values of the program, but the estimated error is smaller than the actual error shown in the program. because ~~at~~ around 1.56 there is a singularity (at $\frac{\pi}{2} \simeq 1.57$) so, the actual relative error is more than $\hbar$. (round off is error is large).

In the richardson' extrapolation method, $\boxed{\text{for } 1^{st} \text{ derivative}}$

- for e^x at $x=0$, we have taken $h=1$ as spacing & we can see clearly from the program that the table converges to 1 with error of 3×10^{-7}.
- For $\tan x$ at $x = 1.56$, the derivative is required at a singularity point so, the results are not so good & but the approximation converges towards the correct value (8579.556). In the program I got 8579.479 which is closer to this value.

$\boxed{\text{For } 2^{nd} \text{ derivative}}$ by this method using ~~dbl~~ float led to huge amount of error so I have used double for it.

- For e^x case the $f''(x)$ converging to 1 in the program.
  For both functions h is used 1.0 & 0.25 respectively.
- For $\tan x$ I got $f''(x) = 1589285.87$ which is closer to the correct value 1589286.

Q3)

Derivatives are required at 1.1, 1.2 .. 1.9 (i.e. interior points)

For 3-point. 1st derivative (from eq → 1 2 3)

$$\text{Truncation error} = \frac{h^2}{6} \times f'''(\xi_c) = \frac{(0.01)^2}{6} \times \frac{2}{x^3} \sim 10^{-4}$$

$[f(x) = \ln x]$

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

$f'''(x) = \frac{2}{x^3}$

$f^{(4)}(x) = \frac{-6}{x^4}$

$f^{(5)}(x) = \frac{24}{x^5}$

$f^{(6)}(x) = \frac{-120}{x^6}$

For 5-point

$$\text{Truncation error} = \frac{h^4}{30} f^{(5)}(\xi_c) = \frac{(0.01)^4}{30} \times \frac{(+2)(-3)(-4)}{x^5} \quad [1 \le x \le 2]$$

$$= \frac{10^{-8}}{30} \times \frac{24}{x^5} \sim 10^{-8}$$

Similar for 2nd derivative also, so the 5-point formula gives more accuracy if there is no round off error (0.01 is too small for 5-point formula).

the optimum spacing is (For 5-point)

1st derivative

from eq → (7)

$$h_{opt} = \left(\frac{45 \hbar M_0}{M_5}\right)^{1/5} = \left(\frac{45 \times (5 \times 10^{-8}) x^5}{24}\right)^{1/5} \quad (\because \hbar M_0 \sim 5 \times 10^{-8})$$

$$\simeq 0.04x$$

2nd derivative

from eq → (11)

$$h_{opt} = \left(\frac{480 \hbar M_0}{M_6}\right)^{1/6} = \cancel{\left(\frac{48 \times (5 \times 10^{-8}) x^4}{81}\right)^{1/4}}$$

$$= \left(\frac{480 \times 5 \times 10^{-8} \times x^6}{120}\right)^{1/6} \simeq 0.075x$$

so, for $x = 1.1$ & 1.9, ~~we can~~ $h > 0.05$ is not possible. we can use extrapolation method for these points.

Q4) $f''(x) = \frac{1}{h^2}\left[a f(x-\frac{3h}{2}) + b f(x-\frac{h}{2}) + c f(x+\frac{h}{2}) + d f(x+\frac{3h}{2})\right]$

using $x=0$

$f(x)=1$ $\quad 0 = \frac{1}{h^2}(a+b+c+d) \Rightarrow 0 = a+b+c+d \rightarrow$ (I)

$f(x)=x$ $\quad \frac{1}{h^2}\left[-\frac{3ah}{2} - \frac{bh}{2} + \frac{ch}{2} + \frac{3dh}{2}\right] \Rightarrow 3a+b-c-3d=0$ — (II)

$f(x)=x^2$ $\quad 2 = \frac{1}{h^2}\left[\frac{9h^2}{4}a + \frac{h^2}{4}b + \frac{h^2}{4}c + \frac{9h^2}{4}d\right] \Rightarrow 8 = 9a+b+c+9d$ — (III)

$f(x)=x^3$ $\quad 0 = \frac{1}{h^2}\left[-\frac{27}{8}h^3 a - \frac{h^3}{8}b + \frac{h^3}{8}c + \frac{27}{8}h^3 d\right] \Rightarrow 27a+b-c-27d=0$ — (IV)

(IV) − (II) $\Rightarrow 24a - 24d = 0 \Rightarrow a = d$

$9\times$(I) − (III) $\Rightarrow 8b + 8c = -8 \Rightarrow b+c = -1$

$9\times$(II) − (IV) $\Rightarrow 8b - 8c = 0 \Rightarrow b = c \Rightarrow b = c = -\frac{1}{2}$

from (I) $\quad a - \frac{1}{2} - \frac{1}{2} + d = 0 \Rightarrow a+d = -1$ & $a = d$

$\Rightarrow a = d = -\frac{1}{2}$

so, we get

$$f''(x) = \frac{1}{2h^2}\left(f(x-\tfrac{3h}{2}) + f(x+\tfrac{3h}{2}) - f(x-\tfrac{h}{2}) - f(x+\tfrac{h}{2})\right)$$

error $= e f^4(\xi)$ $\quad [x-\frac{3h}{2} < \xi < x+\frac{3h}{2}]$

$f(x)=x^4 \rightarrow f''(x) = 12x^2$ & $x=0$

$\Rightarrow 0 = \frac{h^4}{2h^2}\left[2\left(\frac{3}{2}\right)^4 + 2\left(\frac{1}{2}\right)^4\right] + 24e$

$24e = -\frac{h^2}{\cancel{2}} \times \frac{\cancel{164}^{\cancel{82}\ 41}}{\cancel{16}\ 8} \Rightarrow e = -\frac{41h^2}{192}$

roundoff error $= \frac{4\epsilon}{2h^2}$ $\quad$ truncation error $= \left|-\frac{41}{192}h^2 M_4\right|$

for optimum spacing: $\frac{\cancel{4}^{2}\epsilon}{2h_{opt}^2} = \frac{41 h_{opt}^2}{192} M_4$

$\Rightarrow h_{opt} = \left(\frac{384\, \epsilon M_0}{41\, M_4}\right)^{1/4}$

Total error bound $= \frac{4\epsilon}{h^2} = \frac{4\epsilon M_0}{h_{opt}^2} = (4\epsilon)\left(\frac{384}{41} M_0 M_4\right)^{1/4}$

Q4)(ii) $f'''(x) = \frac{1}{h^3}\left[a f(x-2h) + b(x-h) + c f(x+h) + d f(x+2h)\right]$

using $x=0$

$f(x) = 1 \quad \Rightarrow a+b+c+d = 0 \rightarrow (1)$

$f(x) = x \quad \Rightarrow 0 = \frac{1}{h^3}\left[-2ah - bh + ch + 2dh\right] \Rightarrow 2a+b-c-2d=0 \rightarrow (2)$

$f(x) = x^2 \quad \Rightarrow 0 = \frac{1}{h^3}\left[4ah^2 + bh^2 + ch^2 + 4dh^2\right] \Rightarrow 4a+b+c+4d=0 \rightarrow (3)$

$f(x) = x^3 \quad \Rightarrow \frac{1}{h^3}\left[-8ah^3 - bh^3 + ch^3 + 8dh^3\right] = 6 \Rightarrow 8a+b-c-8d=6 \rightarrow (4)$

$(3)-(1) \Rightarrow 3a+3d=0 \Rightarrow a=-d$

$(4)-(2) \Rightarrow 6a-6d=-6 \Rightarrow a-d=1 \Rightarrow a=-\frac{1}{2}, d=+\frac{1}{2}$

from (3) $\rightarrow b+c=0 \Rightarrow b=-c$

from (2) $\rightarrow -c-c-1-1=0 \Rightarrow c=-1 \Rightarrow b=1$

so, we get,

$$f'''(x) = \frac{1}{2h^3}\left[-f(x-2h) + 2f(x-h) - 2f(x+h) + f(x+2h)\right] + e f^{(5)}(\xi)$$

$(x-2h < \xi < x+2h)$

(if we put $f(x)=x^4$ it satisfies the formula).

so we choose $f(x)=x^5$, so error is of the form $ef^{(5)}(\xi)$

$$\Rightarrow 0 = \frac{1}{2\cancel{h^3}}\left[32-2-2+32\right]\cancel{h^5}h^2 + 120e$$

$$\Rightarrow \boxed{e = -\frac{h^2}{4}}$$

Round off error $= \dfrac{\epsilon+2\epsilon+2\epsilon+\epsilon}{2h^3} = \dfrac{3\epsilon}{h^3} = \dfrac{3\hbar M_0}{h^3}$

Truncation error $= \left|\dfrac{-h^4}{4}f^{(5)}(\xi)\right|$

for optimum spacing $\Rightarrow \dfrac{3\hbar M_0}{h^3} = \dfrac{h^4}{4}M_5 \Rightarrow h_{opt} = \left(\dfrac{12\hbar M_0}{M_5}\right)^{1/5}$

Error bound $= \dfrac{6\hbar M_0}{h_{opt}^3} = \dfrac{6\hbar M_0}{\left(\dfrac{12\hbar M_0}{M_5}\right)^{3/5}} = \dfrac{6(\hbar M_0)^{2/5} \times (M_5)^{3/5}}{(12^{3/5})}$

Q5) $\dfrac{\partial f(x,y)}{\partial y} = g(x,y)$

$$\Rightarrow \frac{\partial g(x,y)}{\partial x} = \frac{g(x+h,y) - g(x-h,y)}{2h} + e$$

[e can be found by observing the similarity of the relation already derived :- i.e.

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{6} f'''(\xi)$$

$$\Rightarrow \frac{\partial g(x,y)}{\partial x} = \frac{g(x+h,y) - g(x-h,y)}{2h} - \frac{h^2}{6}\frac{\partial^3 g}{\partial x^3}$$

$$= \frac{1}{2h}\left[\frac{f(x+h), y+k) - f(x+h, y-k)}{2k} - \frac{f(x-h,y+k) - f(x-h,y-k)}{2k}\right]$$

$$+ \frac{1}{2h}\left[-\frac{k^2}{6}\frac{\partial^3 f(x+h,y)}{\partial y^3} + \frac{k^2}{6}\frac{\partial^3 f(x-h,y)}{\partial y^3}\right] - \frac{h^2}{6}\frac{\partial^3 g}{\partial x^3}$$

2 error terms

$$\frac{\partial g}{\partial x} = \frac{1}{4hk}\left[f(x+h, y+k) + f(x-h,y-k) - f(x+h,y-k) - f(x-h,y+k)\right]$$

$$- \frac{k^2}{6}\left(\frac{\frac{\partial^3 f(x+h,y)}{\partial y^3} - \frac{\partial^3 f(x-h,y)}{\partial y^3}}{2h}\right)$$

$$- \frac{h^2}{6} \times \frac{\partial^3}{\partial x^3}\left(\frac{\partial f}{\partial y}\right)$$

$$\Rightarrow \frac{\partial^2 f(x,y)}{\partial x \partial y} = \frac{f(x+h,y+k) + f(x-h,y-k) - f(x+h,y-k) - f(x-h,y+k)}{4hk} - \frac{h^2}{6}\frac{\partial^4 f}{\partial^3 x \partial y} - \frac{k^2}{6}\frac{\partial^4 f}{\partial x \partial y^3}$$

(here the 9 points we used are $\rightarrow$ (x,y), $(x, y\pm k)$, $(x\pm h, y)$ and $(x\pm h, y\pm k)$

Hence Proved.