Computational Physics – Problem Set 1

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1 Machine Precision

In my platform(Ubuntu 19.04), the smallest difference between two numbers that the computer can recognizes is the following. For the single precision, when ϵ is less then $5.9604644775390625 \times 10^{-8}$, the error is negligible. For the double precision, when ϵ is less than $1.11022302462515654042 \times 10^{-16}$, the error is negligible. The exponent in the case of double precision is two times larger than the exponent in the case of single precision.

$$\alpha = aldkjf$$
$$\beta = aldskfaj$$

2 Richarsion Extrapolation

The second derivative of $f(x) = xe^x$ at $x = 2$, by using 3-point formula

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

The Richardson extrapolation:

$$f''(x) = D_1(h) \equiv \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + O(h^2).$$

$$f''(x) = D_1\left(\frac{h}{2}\right) \equiv \frac{f(x+\frac{h}{2}) - 2f(x) + f(x-\frac{h}{2})}{\frac{h^2}{4}} + O(\frac{h^2}{4}).$$

$$\Rightarrow D_2\left(\frac{h}{2}\right) \equiv \frac{4D_1(\frac{h}{2}) - D_1(h)}{4-1}$$
$$= \frac{16f(x+\frac{h}{2}) - f(x+h) - 30f(x) + 16f(x-\frac{h}{2}) - f(x-h)}{3h^2} + O(\frac{h^4}{16})$$

Similarly, to obtain $D_3\Big(\frac{h}{4}\Big)$, one computes

$$D_1\Big(\frac{h}{4}\Big) = \frac{f(x+\frac{h}{4}) - 2f(x) + f(x-\frac{h}{4})}{(\frac{h}{4})^2} + O(\frac{h^2}{16}).$$

$$\Rightarrow D_2\Big(\frac{h}{4}\Big) = \frac{4D_1(\frac{h}{4}) - D_1(\frac{h}{2})}{4-1} + O(\Big(\frac{h}{4}\Big)^4).$$

Therefore,

$$D_3\Big(\frac{h}{4}\Big) = \frac{4^2D_2(\frac{h}{4}) - D_2(\frac{h}{2})}{4^2-1} + O(\Big(\frac{h}{4}\Big)^6).$$

In general, for every iteration step i,

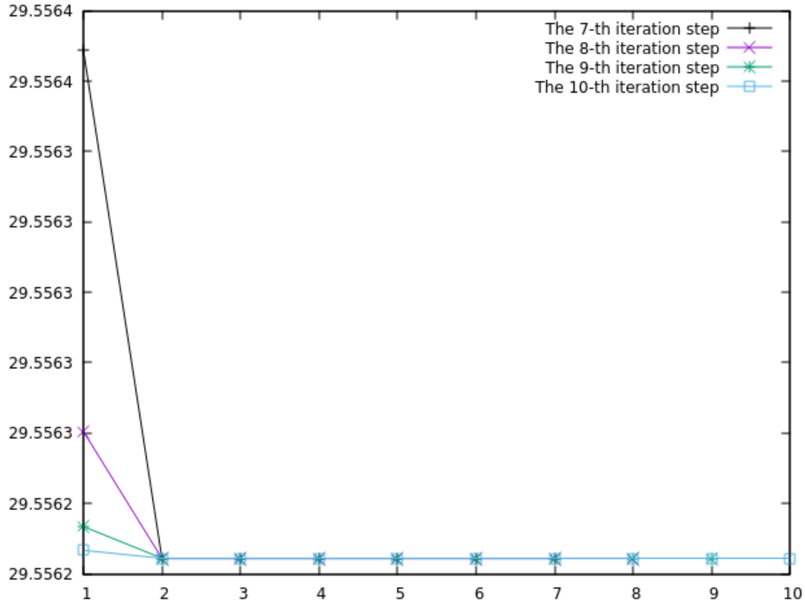
$$D_{i+1}\Big(\frac{h}{2}\Big) = \frac{4^iD_i(\frac{h}{2}) - D_i(h)}{4^i-1}.$$

From the C code, $f''(2)$ is obtained in the various precision shown below:

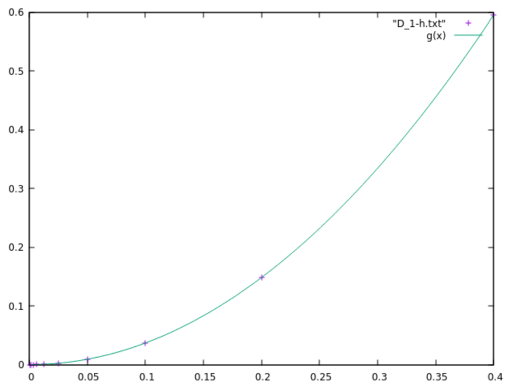
h	D_1	D_2	D_3	D_4	D_5
0.4	30.1515674803				
0.2	29.7042684744	29.5551688058			
0.1	29.5931861000	29.5561586419	29.5562246310		
0.05	29.5654617422	29.5562202895	29.5562243994	29.5562243957	
0.025	29.5585335399	29.5562241391	29.5562243958	29.5562243957	29.5562243957

The exact solution for $f''(x)$ is 29.5562243957.
For $h = \frac{0.4}{2^7}, \frac{0.4}{2^8}, \frac{0.4}{2^9}, \frac{0.4}{2^{10}}$, I plot the values of the second derivative versus different iteration steps. As shown in the following figure, when the iteration steps increases, the values closely approache to the exact solution.

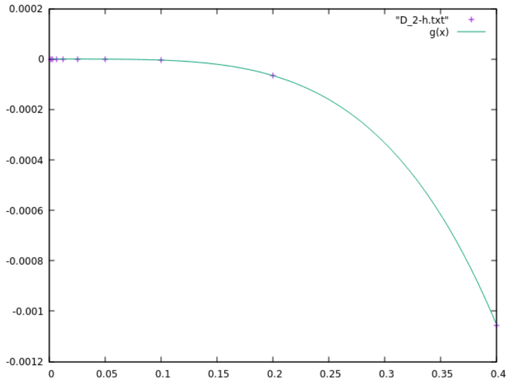
Iteration Steps.png



On the other hand, we can see that $D_1(h)$ decreases at the order of h^2 anad $D_2(h)$ decreases at the order of h^4. The plots below demonstrate this fact.
Below is the plot of $D_1(h) - f''(2)$ versus h and the fitting function $g(x)$ is $3.73618x^2 - 0.00638372x + 7.15812 \times 10^{-5}$



Below is the plot of $D_2(h) - f''(2)$ versus h and the fitting function $g(x)$ is roughly $-0.0414696x^4 + 0.000115702x^3$



It is therefore expected that for $k > 2$, $D_k(h)$ will decrease in the order of h^{2k}. Hence, the computed values will rapidly converge to the desired solution.