# 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 $\epsilon$ is less then $5.9604644775390625 \times 10^{-8}$, the error is negligible. For the double precision, when $\epsilon$ 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.

## 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 $D_3\left(\frac{h}{4}\right)$, one computes

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

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

Therefore,

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

In general, for every iteration step $i$,

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

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.
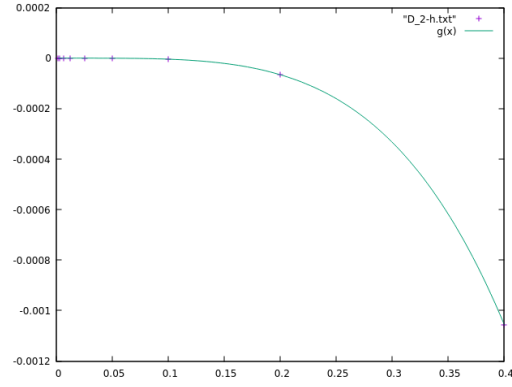
2

Iteration Steps.png
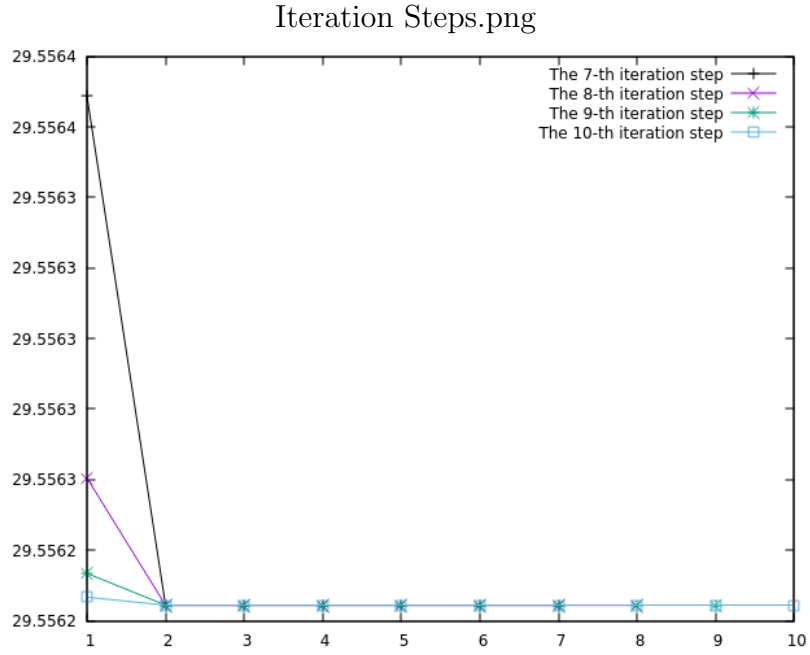


On the other hand, we can see that $D_1(h)$ decreases at the order of $h^2$ anad $D_2(h)$ decreases at the order of $h^4$. The plots below demonstrate this fact.

Below is the plot of $D_1(h) - f''(2)$ versus $h$ and the fitting function $g(x)$ is $3.73618x^2 - 0.00638372x + 7.15812 \times 10^{-5}$
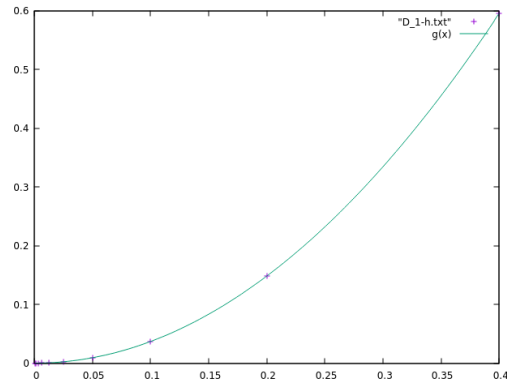
Below is the plot of $D_2(h) - f''(2)$ versus $h$ and the fitting function $g(x)$ is roughly $-0.0414696x^4 + 0.000115702x^3$



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.