Computational Fluid Dynamics (AE 320)

Assignment 1

Submitted By

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Contents

Files Description

All the codes are written in python. This assignment submission contains the following files:

- **README.md** - instructions for running each python code file and the command line arguments to be passed
- **machine_precision.py**: code for computing machine precision/machine epsilon of single and double floating point numbers
- **exp.py**: code for computing exp(x) using taylor series
- **matrix_multiplication.py**: code which computes matrix multiplication of two matrices, if they are compatibe for multiplication
- **input_array.txt**: text file where the matrices for multiplicationn are given as input
- **finite_differences.py**: Code which calculates the derivative of function sin(x) using forward (1st, 2nd and third order), backward (1st, 2nd and third order) and central (2nd and 4th order) difference
- **report.pdf**: This report which discusses the results of the code files.

1 Machine Precision

Machine precision obtained for single and double precision floating point number are as follows:

Single precision (16 bit): 1.19209e-07
Double precision (32 bit): 2.22044604925e-16

2 exp(x) using Taylor series

The algorithm used for evaluating exp(x) starts from 1 and iteratively calculates the successive term till a term becomes 0.

With this algorithm, I am able to evaluate exp(x) for values of x between -714 and 709 (including both these values). Although for negative values, the error is close to 200 percent for $x = -20$ and further rises for negative values with greater magnitude. The error goes to infinity for $x < -373$ (These values have been found analytically by iteratively passing various values of x as a command line argument).

- $x = -5$

  Obtained Value = 0.006737946999084638
  Exact Value = 0.00673794699909
  Error (%) = 1.23063868212e-11
  Number of terms = 254

- $x = -10$

  Obtained Value = 4.539992967040021e-05
  Exact Value = 4.53999297625e-05
  Error (%) = 2.02829927803e-07
  Number of terms = 307

- $x = -50$

  Obtained Value = 2041.8329628976246
  Exact Value = 1.92874984796e-22
  Error (%) = 1.05863026512e+27
  Number of terms = 539

The error is extremely high for exp(-50) although we get close to correct answer for 1/exp(50). This is possibly due to the limitations of precision being reached in dealing with these low numbers (in case of subsequent terms) but the fact we are getting low error for exp(50) and high for exp(-50) suggests the round off error coming into the picture due to cancellation of considerable number of significant digits. This error is further getting propagated on calculations of more terms.

3 Matrix Multiplication

Fairly Straight forward algorithm using nested loops has been implemented. The answer has been verified using np.dot() function.

4 Finite Differences

The formaulas for have been dereived using Taylor Series:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f^{(3)}(x) + \frac{h^4}{4!}f^{(4)}(x) + \frac{h^5}{5!}f^{(5)}(x) \quad \dots$$

4.1 Forward Difference

4.1.1 1st Order

Derivation of first order is straightforward and follows directly from taylor series:

$$f(x+h) = f(x) + hf'(x) + O(h^2)$$

$$\boxed{f'(x) = \frac{f(x+h) - f(x)}{h} + O(h)}$$

4.1.2 2nd Order

For 2nd order, we will need 3 terms - $f(x)$, $f(x+h)$ and $f(x+2h)$.

$$f(x+2h) = f(x) + 2hf'(x) + \frac{(2h)^2}{2!}f''(x) \quad \dots$$

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) \quad \dots$$

Our first derivative can be expressed as:

$$f'(x) = \frac{af(x+2h) + bf(x+h) + cf(x)}{h} + O(h^2)$$

We need to evaluate the coefficients a, b and c such that on substituting the Taylor series expansion of of $f(x+h)$ and $f(x+2h)$ in the above expression, we get $f'(x)$, that is, coefficient of $f'(x) = 1$ and coefficient of $f(x+h)$ and $f(x+2h)$ are 0.

$$f'(x) = \frac{a(f(x) + 2hf'(x) + \frac{(2h)^2}{2!}f''(x)) + b(f(x) + hf'(x) + \frac{h^2}{2!}f''(x)) + c(f(x))}{h} + O(h^2)$$

$$a + b + c = 0$$

$$2a + b = 1$$

$$4a + b = 0$$

On solving for a, b and c:

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

$$b = 2$$

$$c = -\frac{3}{2}$$

So, we get:

$$\boxed{f'(x) = \frac{-f(x+2h) + 4f(x+h) - 3f(x)}{2h} + O(h^2)}$$

4.1.3 3rd Order

For 3rd Order, we will need 4 terms - $f(x)$, $f(x+h)$, $f(x+2h)$ and $f(x+3h)$

Our first derivative can be expressed as:

$$f'(x) = \frac{af(x+3h) + bf(x+2h) + cf(x+h) + df(x)}{h} + O(h^3)$$

Again, I will substitute the Taylor series expansion of $f(x+3h)$, $f(x+2h)$ and $f(x+h)$ and equate coefficient of $f'(x)$ to 1 and other terms to 0.

$$f'(x) = \frac{a[f(x) + 3hf'(x) + \frac{(3h)^2}{2!}f''(x) + \frac{(3h)^3}{3!}f^{(3)}(x)] + b[f(x) + 2hf'(x) + \frac{(2h)^2}{2!}f''(x) + \frac{(2h)^3}{3!}f^{(3)}(x)]}{h} +$$

$$\frac{[f(x) + hf'(x) + \frac{h^2}{2!}f''(x)] + df(x)}{h} + O(h^3)$$

$$a + b + c + d = 0$$

$$3a + 2b + c = 2$$

$$9a + 4b + c = 0$$

$$27a + 8b + 6c + d = 0$$

On solving the above 4 equations, we get:

$$a = \frac{1}{3}$$
$$b = -\frac{3}{2}$$
$$c = 3$$
$$d = -\frac{11}{6}$$

So, we get:

$$f'(x) = \frac{2f(x+3h) - 9f(x+2h) + 18f(x+h) - 11f(x)}{6h} + O(h^3)$$

4.2 Backward Difference

4.2.1 1st Order

Derivation of first order is similar to what :

$$f(x-h) = f(x) - hf'(x) + O(h^2)$$

$$f'(x) = \frac{f(x) - f(x-h)}{h} + O(h)$$

4.2.2 2nd Order

Again we will follow similar procedure as we did with forward difference. We will use $f(x)$, $f(x-h)$ and $f(x-2h)$ to form backward difference. We can write $f'(x)$ as follows:

$$f'(x) = \frac{af(x) + bf(x-h) + cf(x-2h)}{h}$$

Taylor series expansion of $f(x-h)$ and $f(x-2h)$ can be written as -

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!}f''(x) + O(h^3)$$

$$f(x-2h) = f(x) - 2hf'(x) + \frac{(2h)^2}{2!}f''(x) + O(h^3)$$

So our expression for $f'(x)$ becomes as follows:

$$f'(x) = \frac{af(x) + b[f(x) - hf'(x) + \frac{h^2}{2!}f''(x)] + c[f(x) - 2hf'(x) + \frac{(2h)^2}{2!}f''(x)]}{h} + O(h^2)$$

Once again equating coefficients of $f(x)$ anf $f''(x)$ to 1 and coefficient of $f(x)$ to 0, we get three equation as follows:

$$a + b + c = 0$$

$$-b - 2c = 1$$

$$b + 4c = 0$$

On solving the above three equations, we get:

$$a = \frac{3}{2}$$

$$b = -2$$

$$a = \frac{1}{2}$$

So our first derivative expression becomes:

$$f'(x) = \frac{3f(x) - 4f(x-h) + f(x-2h)}{2h} + O(h^2)$$

4.2.3 3rd Order

For 3rd order, we can write the first derivative expression as:

$$f'(x) = \frac{af(x) + bf(x-h) + cf(x-2h) + df(x-3h)}{2h} + O(h^3)$$

Substituting the taylor series expansion of $f(x-h)$, $f(x-2h)$ and $f(x-3h)$ and solving for coefficients, we get the equations as follows:

$$a + b + c + d = 0$$

$$-b - 2c - 3d = 1$$

$$b + 4c + 9d = 0$$

$$b + 8c + 27d = 0$$

On solving these equations, we get:

$$a = 2$$
$$b = -\frac{7}{2}$$
$$c = 2$$
$$d = -\frac{1}{2}$$

So our first derivative expression becomes:

$$\boxed{f'(x) = \frac{4f(x) - 7f(x-h) + 4f(x-2h) - f(x-3h)}{2h} + O(h^3)}$$

4.3 Central Difference

4.3.1 2nd Order

As per Taylor Series:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f^{(3)}(x) + \frac{h^4}{4!}f^{(4)}(x) + \frac{h^5}{5!}f^{(5)}(x) \quad \ldots$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!}f''(x) - \frac{h^3}{3!}f^{(3)}(x) + \frac{h^4}{4!}f^{(4)}(x) - \frac{h^5}{5!}f^{(5)}(x) \quad \ldots$$

So 2nd order central difference formula for 1st derivative can be obtained by simply subtracting the above the equations.

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

4.3.2 4th Order

For 4th order, we will need 5 terms in order to equate the coefficients of terms up to $f^{(5)}(x)$.

So, we can express our first derivative as:

$$f'(x) = \frac{af(x+2h) + bf(x+h) + cf(x) + df(x-h) + ef(x-2h)}{h}$$

Following taylor series expansion:

$$f(x+2h) = f(x) + 2hf'(x) + \frac{(2h)^2}{2!}f''(x) + \frac{(2h)^3}{3!}f^{(3)}(x) + \frac{(2h)^4}{4!}f^{(4)}(x) + \quad \ldots$$

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f^{(3)}(x) + \frac{h^4}{4!}f^{(4)}(x) + \quad \ldots$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!}f''(x) - \frac{h^3}{3!}f^{(3)}(x) + \frac{h^4}{4!}f^{(4)}(x) \quad \ldots$$

$$f(x-2h) = f(x) - 2hf'(x) + \frac{(2h)^2}{2!}f''(x) - \frac{(2h)^3}{3!}f^{(3)}(x) + \frac{(2h)^4}{4!}f^{(4)}(x) \quad \ldots$$

Equating coefficient of $f'(x)$ to 1 and other derivative terms to 0, we get 5 equations as follows:

$$a + b + c + d + e = 0$$

$$2a + b - d - 2e = 0$$

$$4a + b + d + 4e = 0$$

$$8a + b - d - 8e = 0$$

$$16a + b + d + 16e = 0$$

On solving these 5 equations, we get:

$$a = -\frac{1}{12}$$
$$b = \frac{8}{12}$$
$$c = 0$$
$$d = -\frac{8}{12}$$
$$e = \frac{1}{12}$$

So we get:

$$f'(x) = \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h} + O(h^4)$$

4.4 Graphs

The following graphs have been drawn by varying dx from every integer power of 2 from 0 to -30.

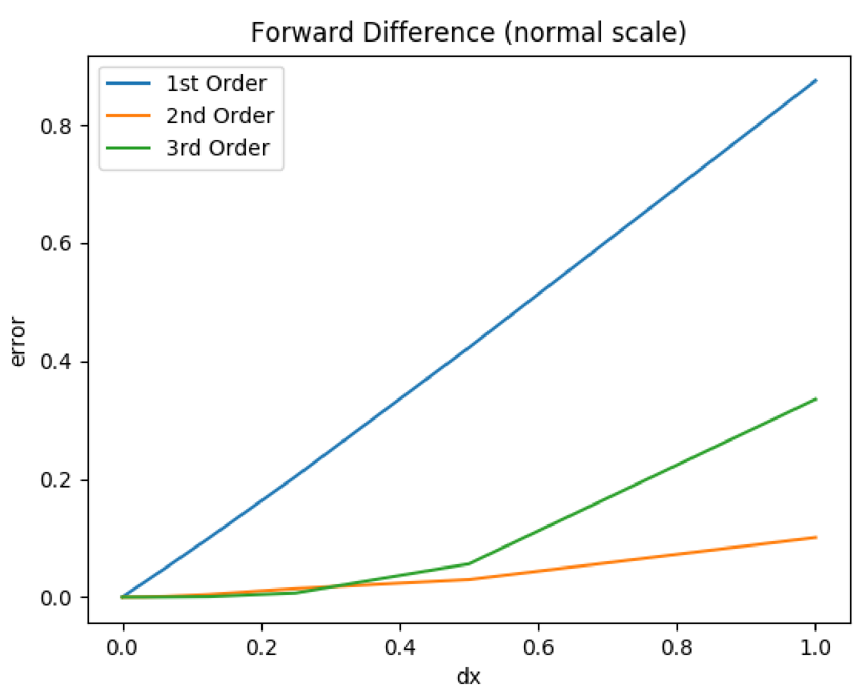

Figure 1: Error reduces on increasing the order of approximation. Initially 2nd order provides the least error but 3rd order overtakes that on further decreasing dx.

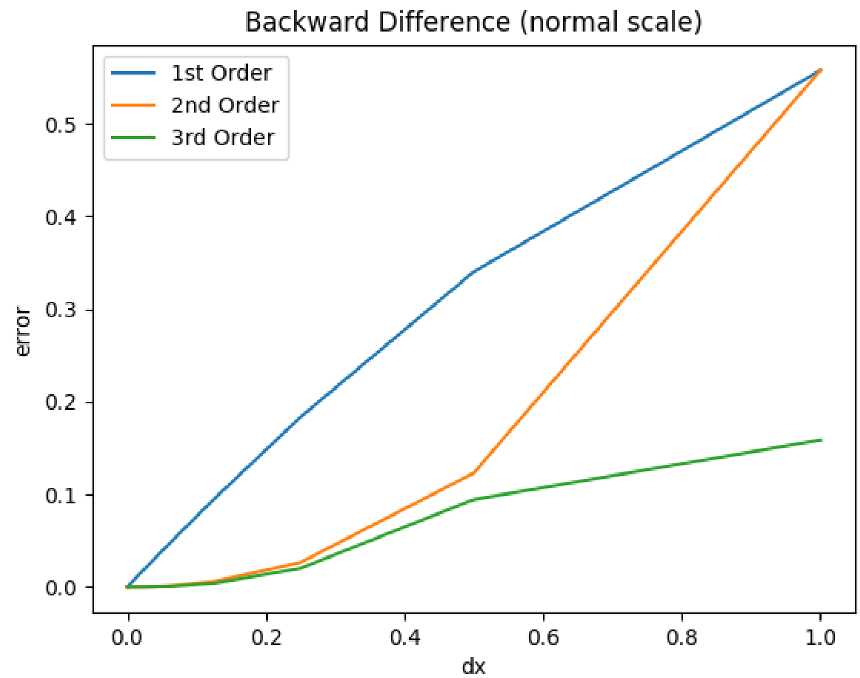

Figure 2: Error reduces on increasing the order of approximation

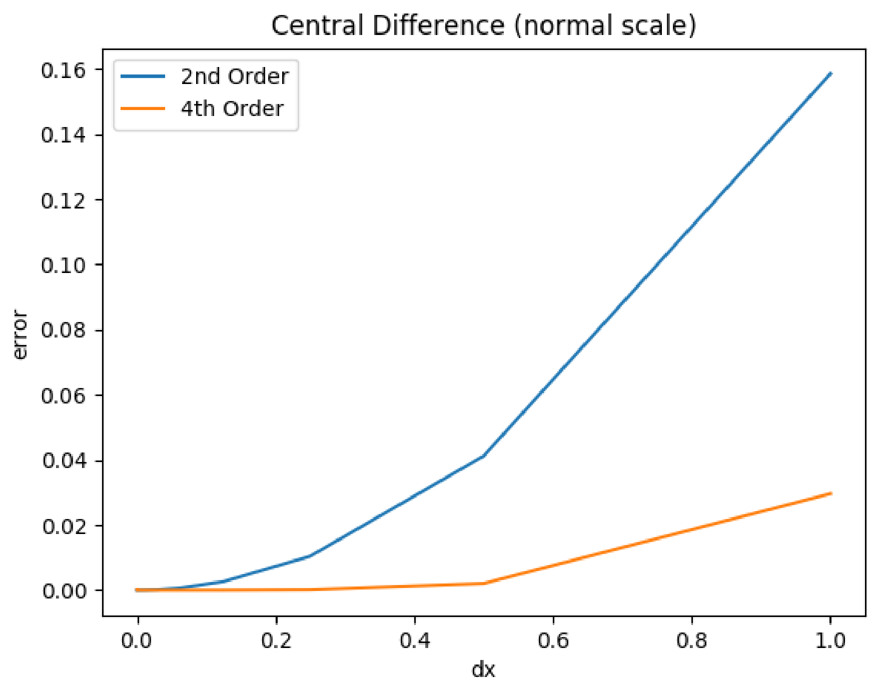

Figure 3: 4th order approximation has significantly less error on greater value of dx but the difference at reduced value is not very clear. This difference is demonstrated well in log-log scale.

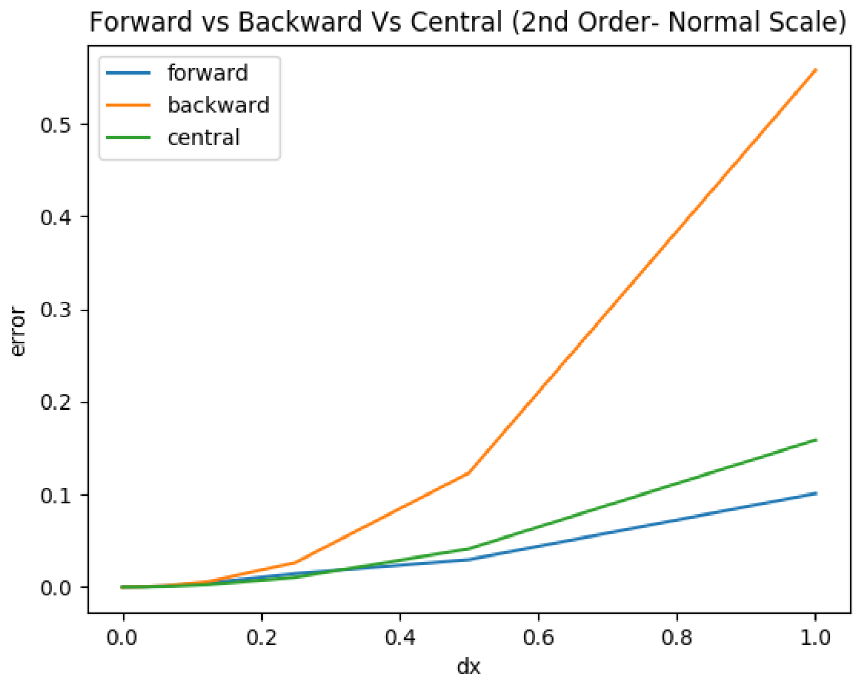

Figure 4: Comparison of 2nd order approximation for forward, backward and central formula. For comparatively larger values of dx, backward difference has largest error while forward has least.

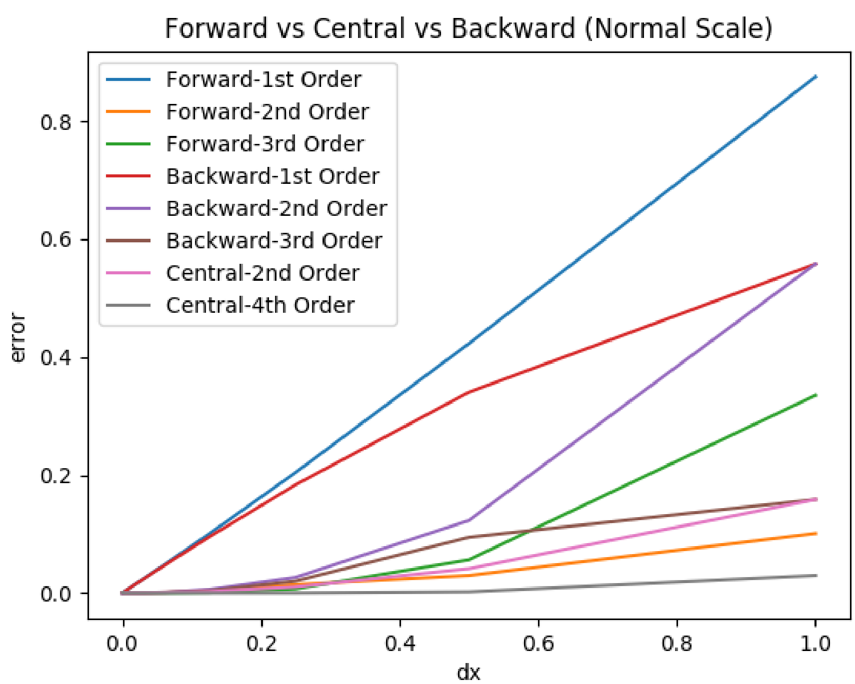

Figure 5: Comparison of all the formulas.

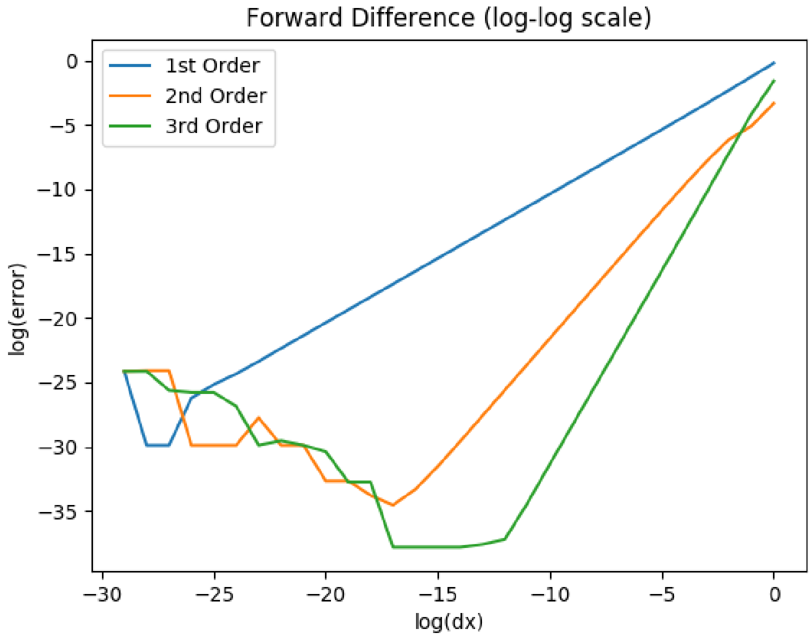

Figure 6: The difference between different much more evident for smaller values of dx. We see random fluctuations below a certain value of dx due to round-off error dominating the truncation error.

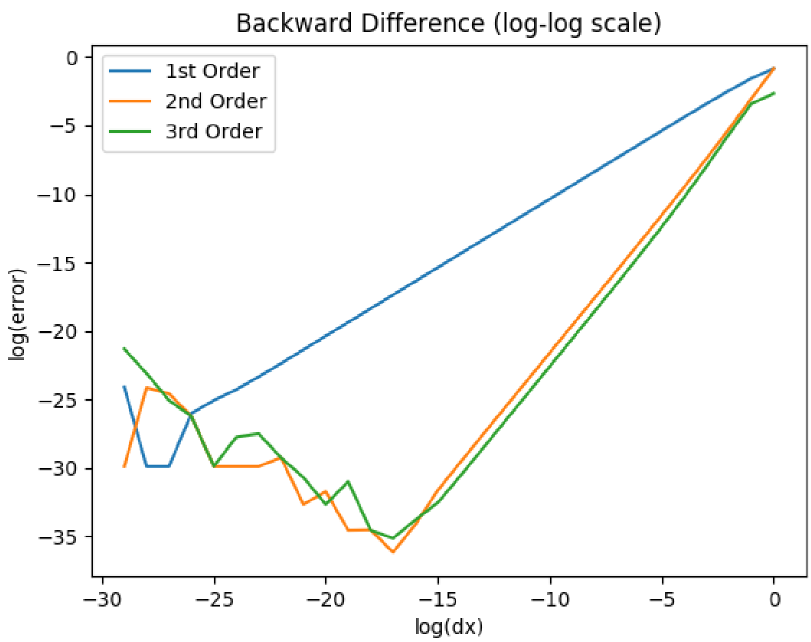

Figure 7: Difference between 2nd and 3rd order is not so much in this case.

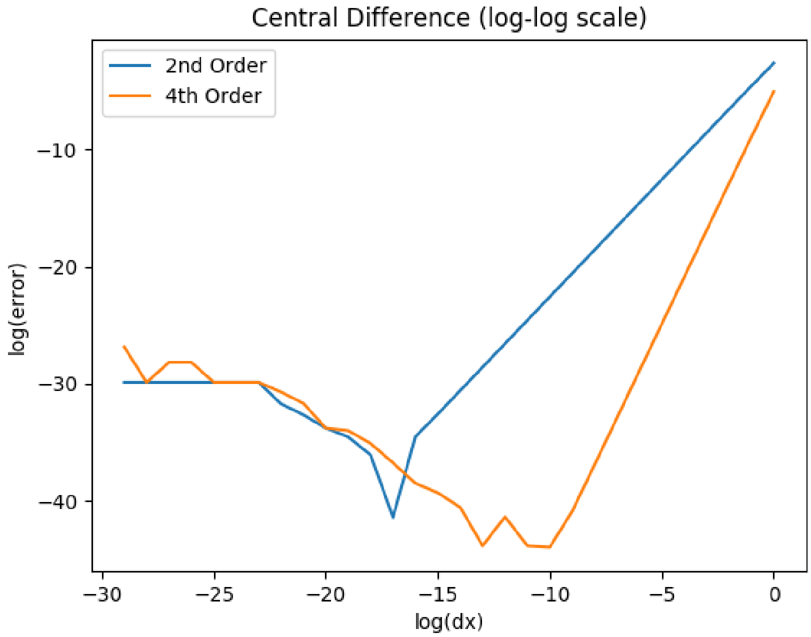

Figure 8: Before the domination of round-off error, 4th order has significantly less error than 2nd order.

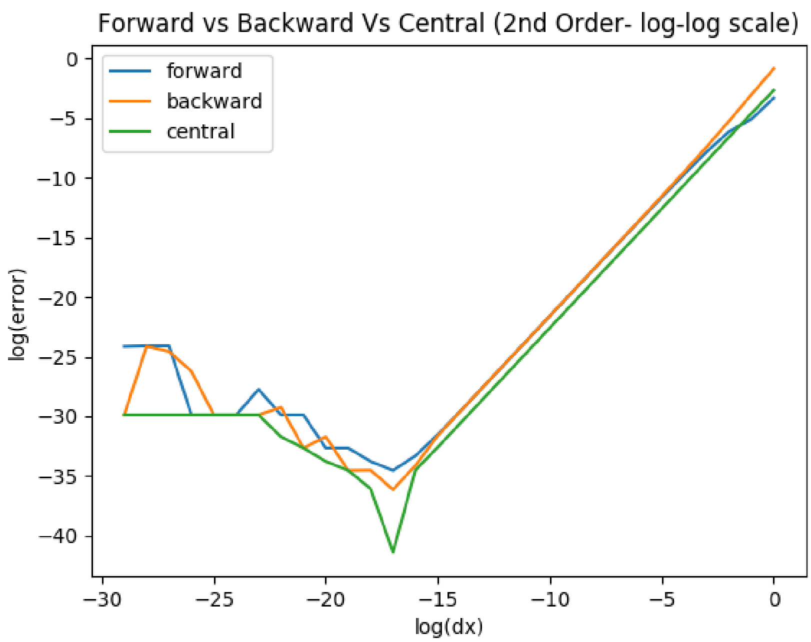

Figure 9: Comparison of forward, central and backward difference of same order

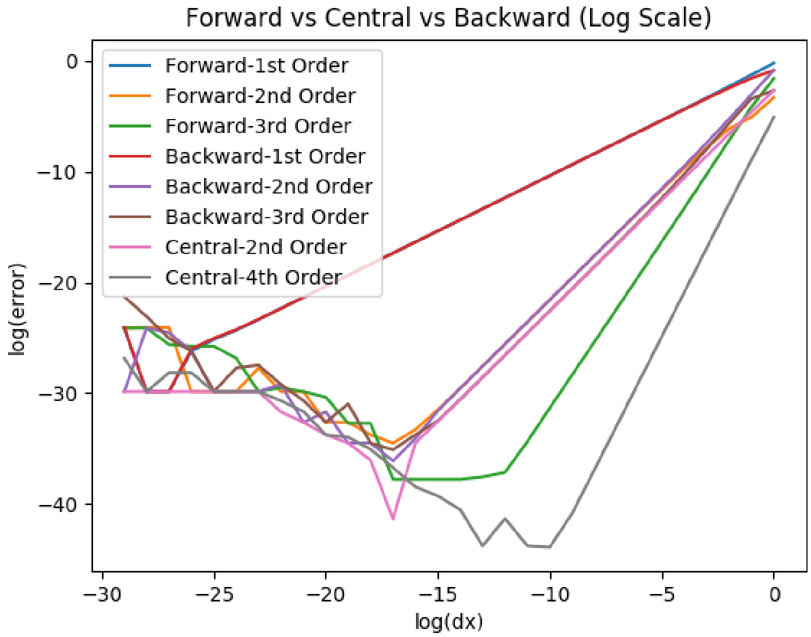

Figure 10: Round-off error kicks earliest in case of central difference 4th order followed by third order approximations demonstrating a trade-off between the precision of approximation and error obtained with respect to the actual error.

4.5 Conclusion

On looking at the graphs, we see a very interesting property of the variation of error with dx. On starting with 1, the error is large. As expected the error decreases on decreases dx as the error is a polynomial function of dx in case of order 1, $(dx)^2$ in case of order 2, $(dx)^3$ in case of order 3 and $(dx)^4$ in case of order 4. So, magnitude of error decrease as we decrease error and moreover the rate of decrease of error is higher for higher order approximations as $(dx)^n$ is less than dx for $dx < 1$ and $n > 1$.

But below a certain value of dx, the error starts increasing and shows fluctuations. It is at this value that the round-off error starts kicking in. We are taking the difference of terms such as $f(x + dx)$ and $f(x)$. For very small values of dx, these two terms share considerable number of significant digits. These common digits are eliminated by the subtraction to leave the difference. The smaller the dx, greater the number of significant digits that are lost.

The error that I talked about in the first paragraph of the conclusions is the truncation error. On log scale, the truncation error reduces with slope that is the order of the formula used to evaluate the derivative, whereas from Taylor series:

$$f(x + dx) = f(x) + f'(x)dx \ldots$$

$f(x + dx)$ approaches $f(x)$ with rate of $f'(x)$. As we are dealing with relative error, the slope of round-off error is effectively 1. Hence, when the truncation error intersects the line with negative unit slope, the round-off error dominates the truncation error.

So once round-off error equals or exceeds the truncation error, for every bit in the representation of dx that we reduce, we lose one bit in the relative error in the derivative.