Numerical Analysis and Computational Physics PHN 311, 2023
Dept. of Physics, IIT Roorkee

Assignment: Numerical derivative

1. **Truncation error in derivative**
Calculate the derivative of f(x) = sin(x) numerically with the following truncation formula

i) single sided difference quotient $$\frac{\mathrm{d}f}{\mathrm{d}x} \approx \frac{f(x+h)-f(x)}{h}$$

ii) the symmetrical difference quotient $$\frac{\mathrm{d}f}{\mathrm{d}x} \approx D_h f(x) = \frac{f(x+h)-f(x-h)}{2h}$$

iii) higher order approximations which can be derived using the extrapolation method

$$-\frac{1}{3}D_h f(x) + \frac{4}{3}D_{h/2} f(x)$$
$$\frac{1}{45}D_h f(x) - \frac{4}{9}D_{h/2} f(x) + \frac{64}{45}D_{h/4} f(x)$$

Define the error as the signed difference between the numerical approximation of the derivative and the exact answer. Plot the error as a function of the step width h on a log-log plot.

2. Use forward- and central-difference algorithms to differentiate the functions cos t and e^t at t = 0.1, 1.0, and 100.

a. Print out the derivative and its relative error E as functions of h. Reduce the step size h until it equals machine precision h ≈ m .

b. Plot log10 |E| versus log10 h and check whether the number of decimal places obtained makes sense.

3. Calculate the second derivative of cos t using the central-difference algorithms. Test it over four cycles, starting with h ≈ π/10 and keep reducing h until you reach machine precision.

4. Plot the following functions in the interval [- π: π], and compute numerical derivatives in each case using forward, backward and central difference formulas. Determine which method gives the most accuracy in each case.

(i) f(x) = e^x
(ii) f(x) = heaviside step function
(iii) f(x) = x
(iv) f(x) = |x|
(v) f(x) = tan(x)
(vi) f(x) = tanh(x)