Ch. 06.
Numerical Differentiation

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AA 2022-2023

Finite Difference Method

- Let us suppose that we are looking for the derivative of a function `f(x)` at some given point x.
- Assume that the function f(x) is known at equally spaced point x_i, such that $h = x_{i+1} - x_i$ is the spacing between nodes. Let

$$f_i = f(x_i) \qquad \text{for} \quad i = 0, \ldots, N_x - 1$$

- In order to find the derivative *f' = df/dx*, the most direct method expands the function using a Taylor series in the neighborhood of x_i:

$$f_{i+1} \equiv f(x_i + h) \approx f_i + f_i' h + \frac{f_i''}{2} h^2 + \frac{f_i'''}{3!} h^3 + O(h^4)$$

- Solving for f'_i, we have the *forward difference (FD)* approximation:

$$\boxed{f_i' \approx \frac{f_{i+1} - f_i}{h} - \frac{f_i''}{2} h}$$

- This approximation has an error proportional to *h*: we can make the approximation error smaller by making *h* smaller, yet precision will be lost through the subtractive cancellation on the left-hand side when h is too small.

Backward Difference

- Similarly, we could expand $f(x_i\text{-}h)$:

$$f_{i-1} \equiv f(x_i - h) \approx f_i - f_i' h + \frac{f_i''}{2} h^2 - \frac{f_i'''}{3!} h^3 + O(h^4)$$

and obtain the *backward difference (BD)* approximation

$$\boxed{f_i' \approx \frac{f_i - f_{i-1}}{h} + \frac{f_i''}{2} h}$$

which still has the same error $O(h)$.

- Both the forward and backward approximations are only first-order accurate and would give the correct answer only when $f(x)$ is a linear function.
- For a quadratic function $f(x)=a+bx^2$, for instance, the forward derivative approximation would result in

$$\frac{f_{i+1} - f_i}{h} = 2bx_i + bh$$

- If you compare it with the exact derivative ($f' = 2bx$), this clearly becomes a good approximation only for small h ($h << 2x_i$)

Central Difference

- Now consider both the right and left expansions:

$$\begin{cases} f_{i+1} \approx f_i + f_i' h + \frac{f_i''}{2} h^2 + \frac{f_i'''}{3!} h^3 + O(h^4) \\ f_{i-1} \approx f_i - f_i' h + \frac{f_i''}{2} h^2 - \frac{f_i'''}{3!} h^3 + O(h^4) \end{cases}$$

- Subtracting the two equations yields the *central difference (CD)* approximation

$$\boxed{f_i' = \frac{f_{i+1} - f_{i-1}}{2h} - \frac{f'''}{6} h^2}$$

- During the subtraction, even powers cancel and our approximation is thus second-order accurate: you can expect the cd approximation to be exact for a parabola.

- The FD, BD and CD approximations are quite natural in the sense that they are reminiscent of the incremental ratio used in elementary calculus.

Higher Order Formulas

- It is possible to obtain higher-order approximation by including more points.

- If we now expand also f_{i+2} and f_{i-2}, we obtain a system of equations

$$\begin{cases} f_{i+2} & \approx & f_i + 2f_i'h + \dfrac{f_i''}{2}(2h)^2 + \dfrac{f_i'''}{3!}(2h)^3 + O(h^4) \\ f_{i+1} & \approx & f_i + f_i'h + \dfrac{f_i''}{2}h^2 + \dfrac{f_i'''}{3!}h^3 + O(h^4) \\ f_{i-1} & \approx & f_i - f_i'h + \dfrac{f_i''}{2}h^2 - \dfrac{f_i'''}{3!}h^3 + O(h^4) \\ f_{i-2} & \approx & f_i - 2f_i'h + \dfrac{f_i''}{2}(2h)^2 - \dfrac{f_i'''}{3!}(2h)^3 + O(h^4) \end{cases}$$

- Getting rid of terms up the fourth derivative, we obtain

$$\boxed{f_i' \approx \frac{f_{i-2} - 8f_{i-1} + 8f_{i+1} - f_{i+2}}{12h} + \frac{h^4}{30}f^{(5)}}$$

which is a fourth-order accurate approximation.

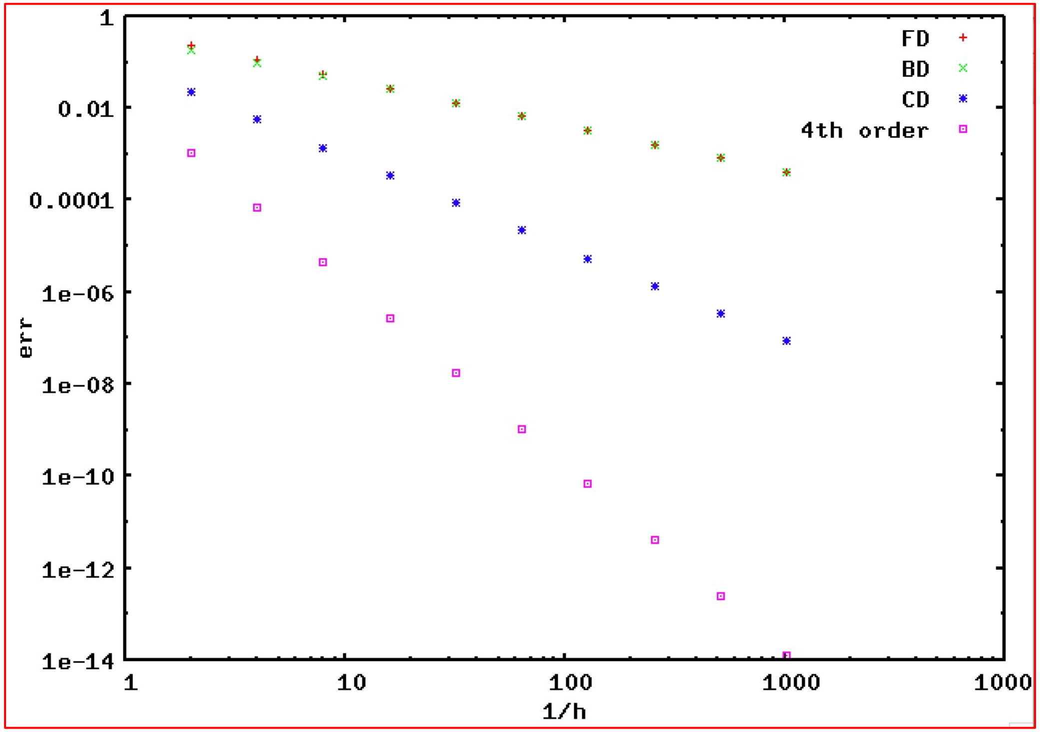
Practice Session #1

- **`derivative.cpp`**: compute the numerical derivative *f(x)=sin(x)* in *x=1* using FD, BD and CD (or higher) using different increments *h=0.5,0.25,0.125, …*

  Plot the error

$$\epsilon = |f'_{\mathrm{num}} - f'_{\mathrm{ex}}|$$

as a function of h using a log-log scaling.



2^{nd}- and Higher-order Derivatives

- For higher order derivatives we can still make use of the Taylor expansion and solve for the second (or higher) derivative.

- From

$$\begin{cases} f_{i+1} & \approx & f_i + f_i'h + \frac{f_i''}{2}h^2 + \frac{f_i'''}{3!}h^3 + O(h^4) \\ f_{i-1} & \approx & f_i - f_i'h + \frac{f_i''}{2}h^2 - \frac{f_i'''}{3!}h^3 + O(h^4) \end{cases}$$

we can solve, e.g., for the 2^{nd} derivative:

$$\boxed{f_i'' \approx \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} + O(h^2)}$$

Practice Session #2

- **`trajectory.cpp`**: Given the particle trajectory

$$x(t) = \alpha t^2 - t^3 \left[1 - exp\left(-\frac{\alpha^2}{t}\right)\right]$$

produce a plot of the velocity and acceleration in the range $0<t<\alpha$.
How many inversion points are present ? (try $\alpha=10$ to begin with)

To this purpose, divide the range `[0, α]` into N equally spaced intervals Δt and use this spacing when computing the derivatives (that is, h = Δt).

Note: central 1st and 2nd derivatives are ill-defined at x = 0. At this point, replace them with the corresponding one-sided approximation (→ next slide).