Computational Physics

Numerical Differentiation

- **Discretization & Finite Differences**
  - **Finite Difference Derivatives**

Discretization & Finite Differences

- consider a smooth function $f(x)$ on the finite interval [a,b] $\in \mathbb{R}$
- Divide interval [a,b] into (N-1) $\in \mathbb{N}$ equally spaced sub-intervals of form $[x_i,x_{i+1}]$, where x_1=a, x_N=b, i.e.

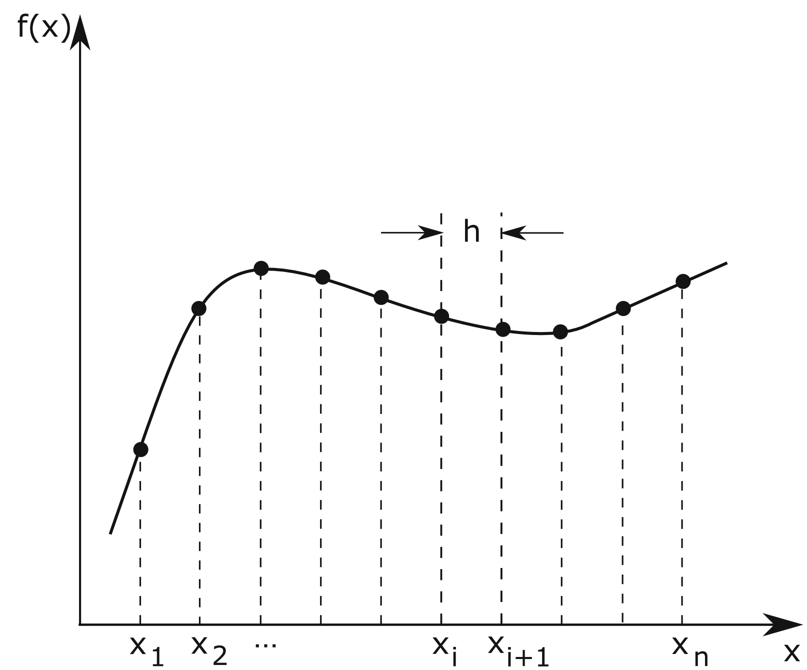
$$x_i = a + (i-1)\frac{b-a}{N-1}, \quad i = 1,\dots,N$$

- Define

$$h = x_{i+1} - x_i = \frac{b-a}{N-1}, \quad \forall i = 1,\dots,N-1$$

(in general h → h_i)

- h should be chosen sufficiently small to approximate $f(x)$ [i.e. some interpolation in $[x_i,x_{i+1}]$ should reproduce $f(x)$ within a required accuracy]
- (in regions of rapid varying of $f(x)$, the grid-spacing should be smaller when using h_i)



Derivatives

- Notation: function $f(x)$ at x_i: $f_i \equiv f(x_i)$
- n-th derivative: [$f^{(0)}(x)=f(x)$]

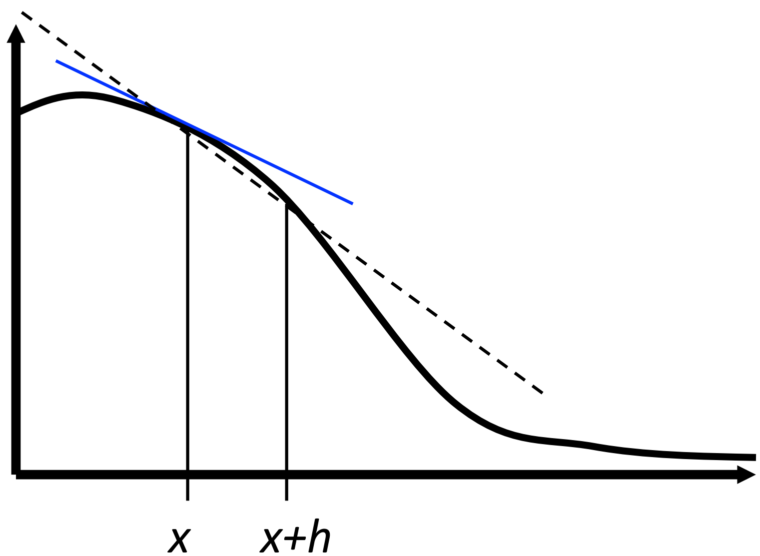
$$f_i^{(n)} \equiv f^{(n)}(x_i) = \left.\frac{\mathrm{d}^n f(x)}{\mathrm{d}x^n}\right|_{x=x_i}$$

- for the first derivate of a smooth function we know:

$$\begin{aligned} f'(x) &:= \lim_{h\to 0} \frac{f(x+h)-f(x)}{h} \\ &= \lim_{h\to 0} \frac{f(x)-f(x-h)}{h} \\ &= \lim_{h\to 0} \frac{f(x+h)-f(x-h)}{2h} \end{aligned}$$

First Derivative

- The mathematical definition: $$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$
- Graphically, as the tangential line:



- Numerically, we can not calculate the limit as *h* goes to zero, so we need to approximate it. [Discreteness of floating point numbers and subtractive cancellation]
- Apply directly for a non-zero *h* leads to the slope of the secant curve.

Taylor series

- If the function *f(x)* is (n-1)-times continuously differentiable on the interval [a, b] then it can be expressed in terms of a series expansion at point $x_0 \in$ [a,b]:

$$f(x) = \sum_{k=0}^{n} \frac{f^{(k)}(x_0)}{k!}(x-x_0)^k + \frac{f^{(n+1)}[\zeta(x)]}{(n+1)!}(x-x_0)^{n+1}, \quad \forall x \in [a,b]$$

truncation error
with $\zeta(x)$ between x and x_0

In third order →
$f_{i+1}=f(x_i+h)$
$f_{i-1}=f(x_i-h)$

$$\begin{aligned} f_{i+1} &= f(x_i) + hf'(x_i) + \frac{h^2}{2}f''(x_i) + \frac{h^3}{6}f'''[\zeta(x_i+h)] \\ &= f_i + hf_i' + \frac{h^2}{2}f_i'' + \frac{h^3}{6}f_{i+\epsilon\zeta}''' \ , \end{aligned}$$

$$f_{i-1} = f_i - hf_i' + \frac{h^2}{2}f_i'' - \frac{h^3}{6}f_{i+\epsilon\zeta}'''$$

Finite Difference Derivatives

- *Difference operators*
  - Forward difference: $\Delta_+ f_i = f_{i+1} - f_i$
  - Backward difference: $\Delta_- f_i = f_i - f_{i-1}$
  - Central difference: $\Delta_c f_i = f_{i+1} - f_{i-1}$

- Forward difference derivative:

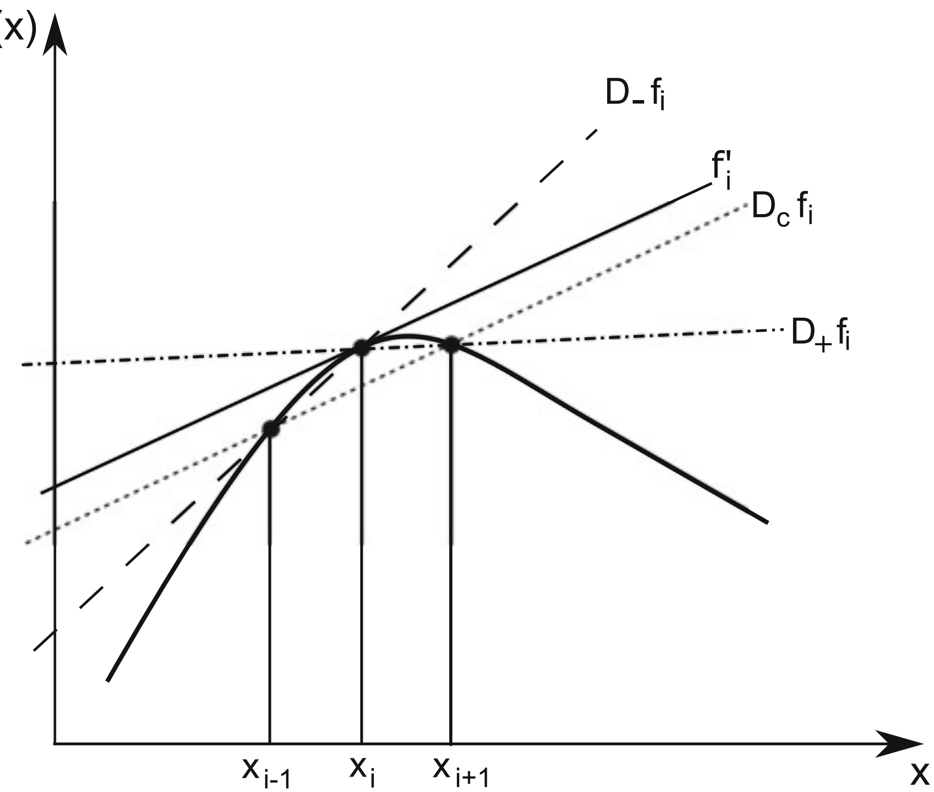
$$D_+ f_i = \frac{\Delta_+ f_i}{h} = \frac{f_{i+1} - f_i}{h}$$

- Backward difference derivative:

$$D_- f_i = \frac{\Delta_- f_i}{h} = \frac{f_i - f_{i-1}}{h}$$

- Central difference derivative:

$$D_c f_i = \frac{\Delta_c f_i}{2h} = \frac{f_{i+1} - f_{i-1}}{2h}$$



…

This gives for the Taylor series:

$$
\begin{aligned}
f_i' &= D_+ f_i - \frac{h}{2} f_i'' - \frac{h^2}{6} f_{i+\epsilon\zeta}''' \\
&= D_- f_i + \frac{h}{2} f_i'' - \frac{h^2}{6} f_{i+\epsilon\zeta}''' \\
&= D_c f_i - \frac{h^2}{6} f_{i+\epsilon\zeta}''' \,.
\end{aligned}
$$

Note: $$D_c = \frac{1}{2}(D_+ + D_-)$$

Reminder: errors

- ***Truncation Error:*** introduced in the solution by the approximation of the derivative
- ***Round-off Error:*** introduced in the computation by the finite number of digits used by the computer

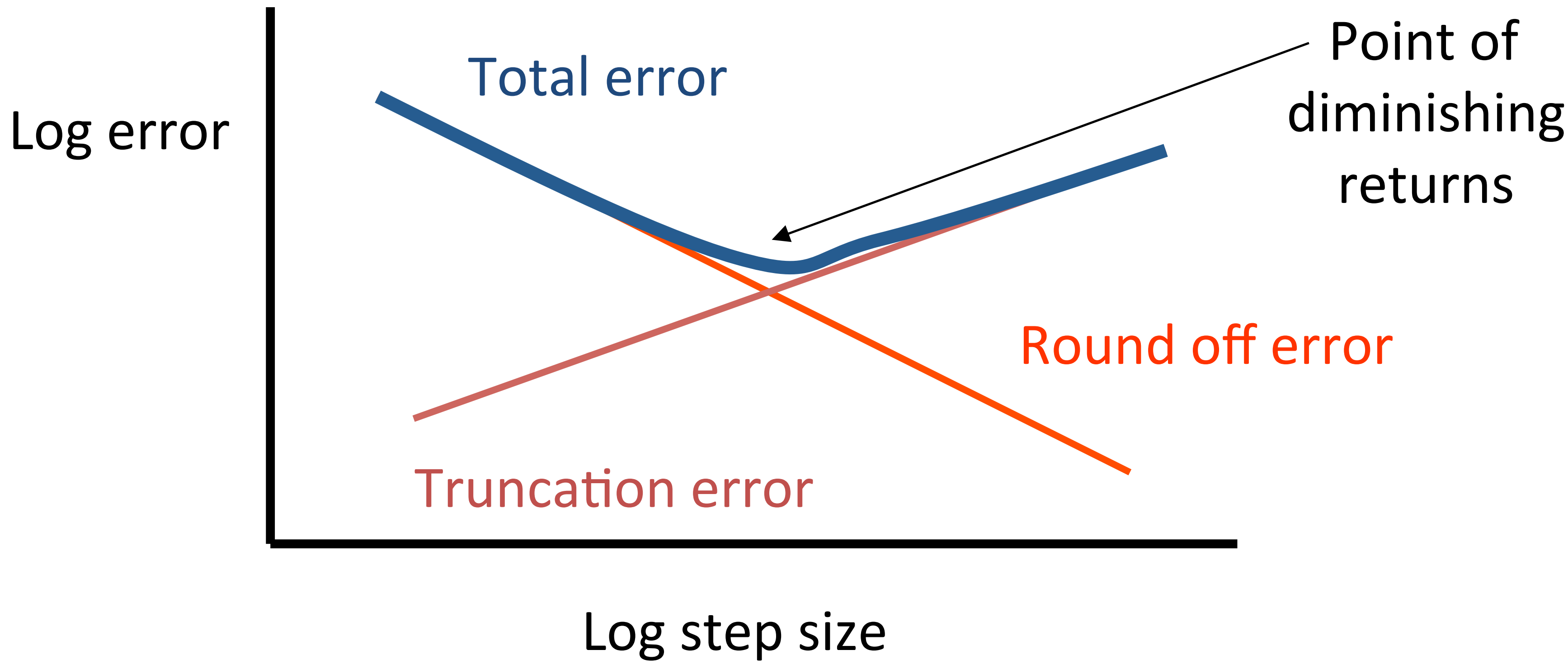
- Solving differential equations is done in multiple steps. Therefore, we also have:
  - ***Local Error:*** from each term of the equation
  - ***Global Error:*** from the accumulation of local error

Truncation errors

- Let $f(x)$ = a, and $f(x+h)$ = a+e.
- Then, as h approaches zero: e<<a.
- With limited precision on our computer, our representation of $f(x) \approx a \approx f(x+h)$.
- We can easily get a random round-off bit as the most significant digit in the subtraction.
- Dividing by h, leads to a very wrong answer for $f'(x)$.

Error trade-off

- Using a smaller step size reduces truncation error.
- However, it increases the round-off error.
- Trade off/diminishing returns occurs: Always think and test!



Multi-point approximations

- Forward and Backward derivates use two points, Central **three** points (f_i cancels).
- Using higher order terms in the Taylor series results in smaller truncation errors:

$$D_+ f_i = f_i' + \frac{h}{2} f_i'' + \frac{h^2}{6} f_i''' + \frac{h^3}{24} f_i^{IV} + \frac{h^4}{120} f_i^V + \dots$$

$$D_- f_i = f_i' - \frac{h}{2} f_i'' + \frac{h^2}{6} f_i''' - \frac{h^3}{24} f_i^{IV} + \frac{h^4}{120} f_i^V \mp \dots$$

$$D_c f_i = f_i' + \frac{h^2}{6} f_i''' + \frac{h^4}{120} f_i^V + \dots$$

- One finds: $$8D_c f_i - D_c f_{i-1} - D_c f_{i+1} = 6f_i' - \frac{h^4}{5} f_{i+\epsilon\zeta}^V$$
- and therefore:

$$f_i' = \frac{1}{6}\left(8D_c f_i - D_c f_{i+1} - D_c f_{i-1}\right) + \frac{h^4}{30} f_i^V$$

$$= \frac{1}{12h}\left(f_{i-2} - 8f_{i-1} + 8f_{i+1} - f_{i+2}\right) + \frac{h^4}{30} f_i^V$$

Read chapter 2.4 for higher order approximations

Example

For a concrete example of the error due to finite difference approximation we look at

$$f(x) = \exp(i\omega x) \qquad x \in \mathbb{R}$$

analytically:

$$f'(x) = i\omega \exp(i\omega x)$$

discretization:

$$x_k = x_0 + kh$$

$$f_k = \exp[i\omega(x_0 + kh)]$$

$$f_k' = i\omega \exp[i\omega(x_0 + kh)] = i\omega f_k$$

Finite difference derivative

$$D_+ f_k = i\omega f_k \exp\left(\frac{ih\omega}{2}\right) \operatorname{sinc}\left(\frac{h\omega}{2}\right)$$

sinc(x)=sin(x)/x

$$D_- f_k = i\omega f_k \exp\left(-\frac{ih\omega}{2}\right) \operatorname{sinc}\left(\frac{h\omega}{2}\right)$$

$$D_c f_k = i\omega f_k \operatorname{sinc}(h\omega)$$

…

To study how good the the finite difference derivates are, we look at its ratio to true derivate:

$$\left|\frac{D_+ f_k}{f'_k}\right| = \left|\frac{D_- f_k}{f'_k}\right| = \mathrm{sinc}\left(\frac{h\omega}{2}\right)$$

$$\left|\frac{D_c f_k}{f'_k}\right| = \mathrm{sinc}(h\omega)$$

- since $|\sin(x)| \leq |x|$ for all x, the approximation always underestimates the derivative since $f(x)$ oscillates and the finite difference derivative implies a linear interpolation.
- for $h\omega$ being multiples of 2π (or π) the finite differences are zero.
  → choose $h \ll 2\pi/\omega$
- Easy to see if analytical form known (then one does not need a finite difference anyway). Typically, even $f(x)$ is not known analytically.
  → h has to be chosen carefully

Partial Derivatives

Works similarity by independently discretizing the function on a regular lattice.

E.g. central difference for mixed derivative of g(x,y):

$$\frac{\partial}{\partial y}\frac{\partial}{\partial x}g(x,y)\bigg|_{(i,j)} = \frac{1}{2h_x}\left[\frac{\partial}{\partial y}g(x,y)\bigg|_{(i+1,j)} - \frac{\partial}{\partial y}g(x,y)\bigg|_{(i-1,j)}\right] + \mathscr{O}(h_x^2)$$

$$= \frac{1}{2h_x}\left[\frac{g_{i+1,j+1}-g_{i+1,j-1}}{2h_y} + \mathscr{O}(h_y^2)\bigg|_{(i+1,j)}\right.$$

$$\left. - \frac{g_{i-1,j+1}-g_{i-1,j-1}}{2h_y} - \mathscr{O}(h_y^2)\bigg|_{(i-1,j)}\right] + \mathscr{O}(h_x^2)\ , \quad ($$

→ $$\frac{\partial}{\partial y}\frac{\partial}{\partial x}g(x,y)\bigg|_{(i,j)} \approx \frac{1}{2h_x}\frac{g_{i+1,j+1}-g_{i+1,j-1}-g_{i-1,j+1}+g_{i-1,j-1}}{2h_y}$$

There are others methods, e.g., the finite element method (FEM): the function is discretized in d-dimensional polytopes or simplexes (elements) and interpolated by polynomials within.

Demo & Homework

Planned schedule for following lectures

- Thursday: Numerical integration, more python
- Next week: The Kepler problem – lecture&lab
- 2/4&6: ODEs – lecture&lab
- 2/11&13: Double Pendulum – lecture&lab
- 2/18&20: Molecular dynamics – lecture&lab
- 2/25&27: 1D stationary heat equation – lecture&lab
- 3/4&6: PDEs – lecture&lab (not topic in midterm
- **spring break**
- 3/18&20: **no class**
- 3/25&27: midterm task + random numbers & Monte Carlo
- 4/1&3: Ising model – lecture&lab
- *April*: final project assignment and preparation
- 4/24: final project presentations