Lecture # 21

03/01/2023

## Doing calculus on computer:

- Numerical differentiation (today)
- " integration (on Fri)
- " solution of ODE initial value problem (the lecture after)

## Computing derivatives on computer:

Overall 3 different approaches

Symbolic derivatives

Example software:

Maple, Mathematica,

MATLAB Symbolic Toolbox

Automatic differentiation

Example software:

AutoDiff

we will not cover these

Exact

Approximate numerical differentiation

Example Algorithms: Finite differences

This class

# Finite difference approximation for $f'(\cdot)$ :

We know a function $f(x)$, $f : \mathbb{R} \mapsto \mathbb{R}$

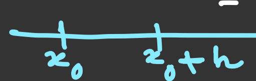
Let $0 < h \underbrace{\ll}_{\text{"much less than"}} 1$

Taylor expansion of $f$ :

$$f(x_0+h) = f(x_0) + h f'(x_0) + \frac{h^2}{2} f''(x_0) + \frac{h^3}{6} f'''(x_0) + \dots \qquad (*)$$

$$\Rightarrow f'(x_0) = \frac{f(x_0+h) - f(x_0)}{h} - \frac{h}{2} f''(x_0) - \frac{h^2}{6} f'''(x_0) - \dots$$

$$\Rightarrow \boxed{f'(x_0) = \frac{f(x_0+h) - f(x_0)}{h} + O(h)}$$



This is called <u>Two Point Forward Difference approximation</u> of $f'(x_0)$

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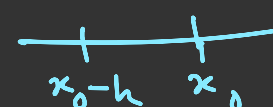
In (*), replacing $h$ by $(-h)$, we get :

$$f(x_0-h) = f(x_0) - h f'(x_0) + \frac{h^2}{2} f''(x_0) - \frac{h^3}{6} f'''(x_0) + \cdots \quad (**)$$

$$\Rightarrow \boxed{f'(x_0) = \frac{f(x_0) - f(x_0-h)}{h} + O(h)}$$

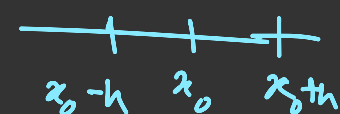
<u>Two point backward difference approximation</u> of $f'(x_0)$



On the other hand, if we do: (*) − (**),
then we get:

$$f'(x_0) = \frac{f(x_0+h) - f(x_0-h)}{2h} - \frac{h^2}{12} f'''(x_0) + \dots$$

$$= \underbrace{\frac{f(x_0+h) - f(x_0-h)}{2h}}_{\text{Two Point Central Difference approximation}} + O(h^2)$$



Example: (Approximating the first derivative)

Given $f(x) = \underbrace{\ln}_{\text{natural log.}}(x)$. Compute $f'(3)$.

Exact:

$$f'(x) = \frac{1}{x} \Rightarrow f'(3) = \frac{1}{3}$$
$$= 0.333\ldots$$
$$= 0.\overline{3}$$

Forward difference:

Say step-size $h = 0.4$

$$f'(3) \approx \frac{\ln(3+0.4) - \ln(3)}{0.4} = \frac{\ln(3.4) - \ln(3)}{0.4}$$
$$\approx 0.31290786$$

Backward difference:

$$f'(3) \approx \frac{\ln(3) - \ln(3-0.4)}{0.4}$$

$$= \frac{\ln(3) - \ln(2.6)}{0.4}$$

$$\approx 0.35775211$$

Central difference:

$$f'(3) \approx \frac{\ln(3.4) - \ln(2.6)}{2 \times 0.4} \approx 0.33532998 .$$

## Approximating $2^{nd}$ derivative $f''(x_0)$ in single dimension:

Adding (*) and (**), we get:

$$f(x_0+h) + f(x_0-h) = 2f(x_0) + h^2 f''(x_0) + \frac{h^4}{12} f''''(x_0) + \cdots$$

$$\Rightarrow \quad f''(x_0) = \underbrace{\frac{f(x_0+h) - 2f(x_0) + f(x_0-h)}{h^2}}_{\text{Three point central difference approximation for } f''(x_0)} + O(h^2)$$

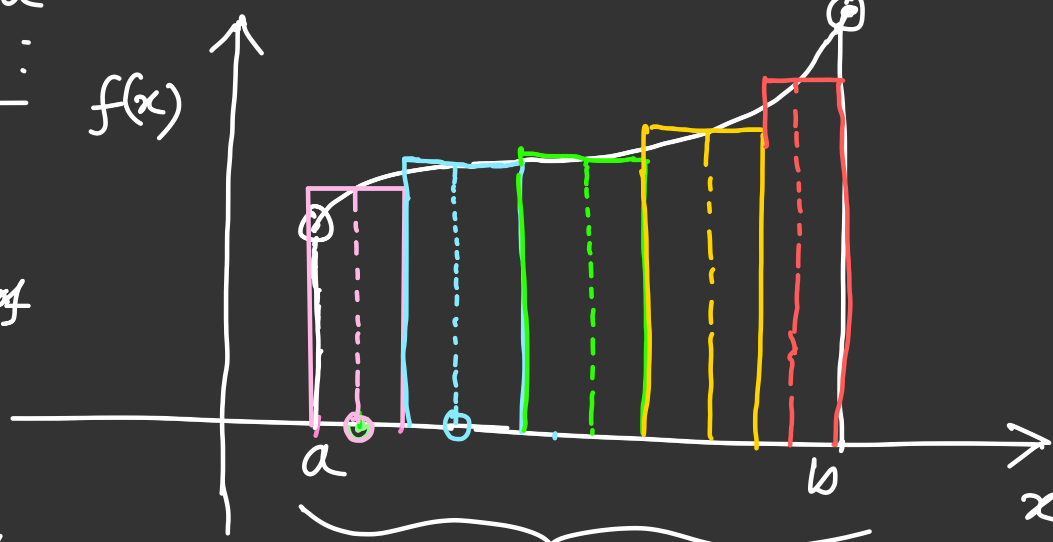
# Numerical Integration

Approximating $\int_a^b f(x)\,dx$

## Midpoint method :

Area of a rectangle

= width of the partition/sub-interval × height of the midpoint of that partition




$\int_a^b f(x)\,dx \approx$ sum of the areas of these rectangular slices