PH 3120 – Computational Physics Laboratory I

Numerical Differentiation and Integration

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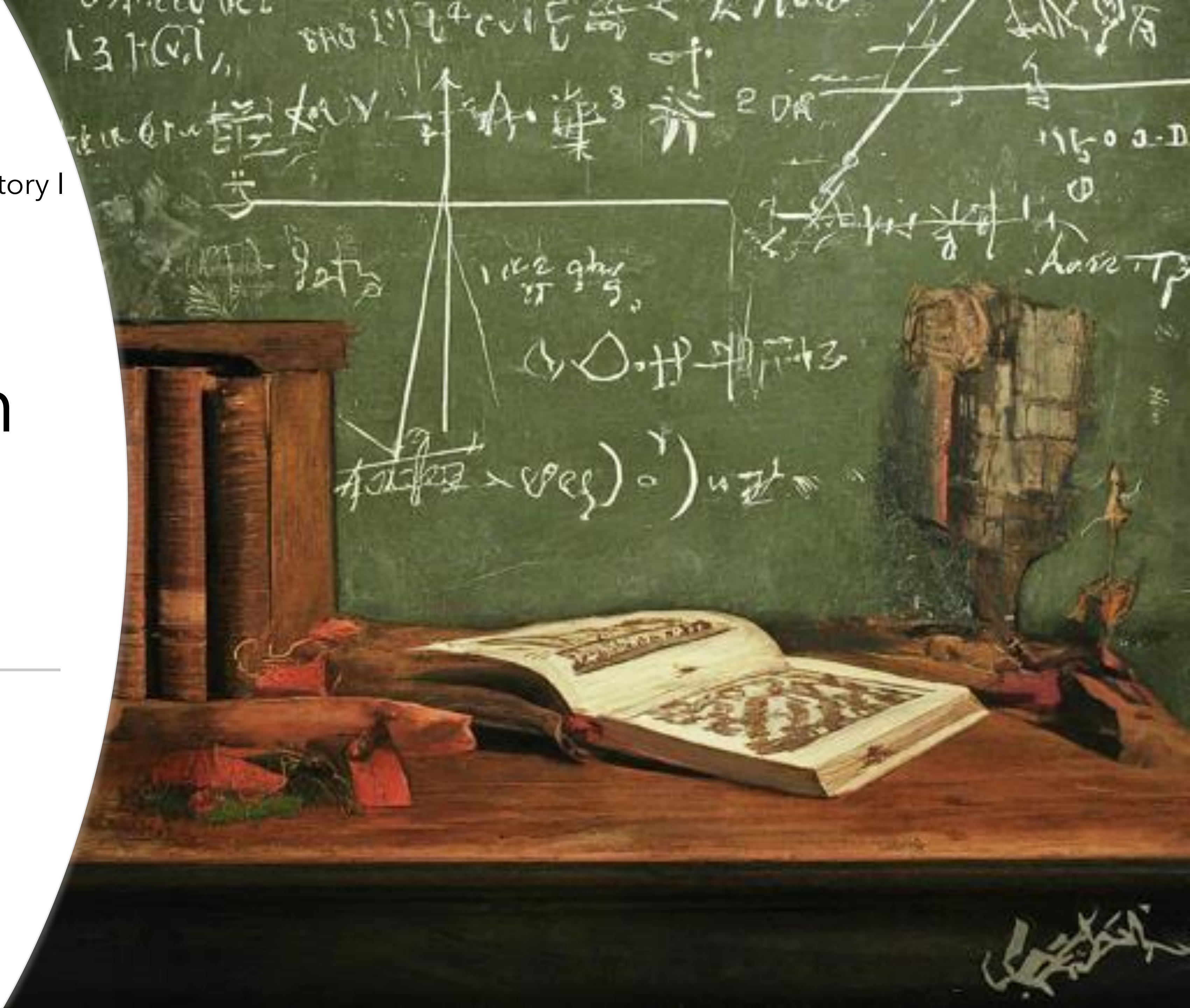


First Derivative in Physics

- The first derivative of a function represents the rate at which the function changes.
- In physics, this concept is fundamental in understanding motion, forces, and various other phenomena.

Example:

Velocity: The first derivative of the position $x(t)$ with respect to time t is the velocity $v(t) = \frac{dx}{dt}$.

Force: According to Newton's second law, the force F is related to the acceleration a ($a = \frac{dv}{dt}$) by $F = ma$.

Numerical Differentiation

Numerical differentiation is the process of estimating the derivative of a function using discrete data points.

Finite Difference Methods

Finite difference methods approximate the derivative of a function using finite differences.

There are three common finite difference approximations:

Forward Difference	Backward Difference	Central Difference
$f'(x) \approx \frac{f(x+h) - f(x)}{h}$	$f'(x) \approx \frac{f(x) - f(x-h)}{h}$	$f'(x) \approx \frac{f(x+h) - f(x-h)}{h}$

In the above expressions, h is a small step size.

Numerical Differentiation

Finite Difference Methods

Consider a function $f(x) = \sin(x)$. We want to estimate its derivative at $x = \pi/4$ using a small step size $h = 0.001$.

Forward Difference	Backward Difference	Central Difference
$f'(x) \approx \dfrac{f(x+h) - f(x)}{h}$	$f'(x) \approx \dfrac{f(x) - f(x-h)}{h}$	$f'(x) \approx \dfrac{f(x+h) - f(x-h)}{h}$
$f'(x) \approx \dfrac{\sin(\frac{\pi}{4} + 0.001) - \sin\left(\frac{\pi}{4}\right)}{0.001}$	$f'(x) \approx \dfrac{\sin\left(\frac{\pi}{4}\right) - \sin\left(\frac{\pi}{4} - 0.001\right)}{0.001}$	$f'(x) \approx \dfrac{\sin\left(\frac{\pi}{4} + 0.001\right) - \sin\left(\frac{\pi}{4} - 0.001\right)}{0.001}$
$f'(x) = 0.707$	$f'(x) = 0.7071$	$f'(x) = 0.7071$

Using the analytical methods, we can show that

$$f'(x) = \frac{d\sin(x)}{dx} = \cos(x) \;\rightarrow\; f'\left(\frac{\pi}{4}\right) = \cos\left(\frac{\pi}{4}\right) = \frac{1}{\sqrt{2}} = 0.7071067$$

Taylor Series

The Taylor series is a mathematical technique used to approximate functions that are difficult or impossible to express in closed form.

It represents a function as an infinite sum of terms calculated from the values of its derivatives at a single point.

$$f(x) = \sum_{n=0}^{\infty} \frac{f^n(a)}{n!}(x-a)^n$$

$$f(x) = f(a) + f'(a)(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \frac{f'''(a)}{3!}(x-a)^3 + \cdots$$

Here, $f'(a), f''(a),$ and higher-order derivatives are evaluated at a.

Derivation of the Forward Finite Difference Method

Consider the Taylor series expansion of $f(x+h)$ around x:

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

To isolate $f'(x)$, we rearrange the Taylor series expansion:

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

Divide through by h:

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

For a sufficiently small h, the higher-order terms (i.e., terms involving h^2, h^3, etc.) become negligible.

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

Truncation Error

The truncation error refers to the inherent inaccuracy introduced when using the forward difference method to approximate the derivative of a function.

It arises because we replace the infinite Taylor series expansion of the derivative with a finite number of terms.

The following is the general equation of the Taylor Equation around x.

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

Assume that we approximate $f(x+h)$ up to the h^2 term. We can rewrite the above expression as

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

Therefore, the approximated value is given by

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

Truncation Error

Truncation error $(TE)$is given by

$$TE = \text{Exact Value} - \text{Approximate Value}$$

$$TE = \frac{f'''(x)}{3!}h^3 + \frac{f''''(x)}{4!}h^4 + \cdots$$

Order of Accuracy

The order of accuracy of a numerical method indicates how the truncation error decreases as the step size h decreases.

If the leading term of the truncation error is proportional to h^p, the method is said to be of order p.

That is denoted by $O(h^p)$

For the above example, the order of accuracy is 3 which is indicated by $O(h^3)$.

Truncation Error of Forward Difference Method

The truncation error of the forward difference method arises due to the approximation of the derivative of a function.

$$\boxed{f(x+h) = f(x) + f'(x)(h) + \frac{f''(x)}{2!}h^2 + \frac{f'''(x)}{3!}h^3 + \cdots}$$

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

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

Truncation error is given by

$$TE = \frac{f''(x)}{2!}h + \frac{f'''(x)}{3!}h^2 + \cdots$$

Therefore, TE is of the order of $O(h)$

Trapezoidal Rule

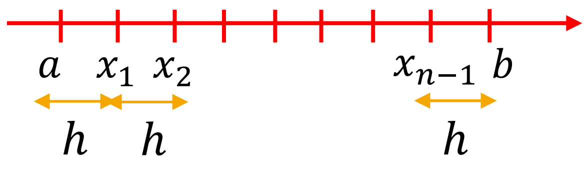
The Trapezoidal Rule is a numerical method for approximating the definite integral of a function.

The following expression provides the approximation of integral of the function $f(x)$ from a to b

with respect to the variable x.

$$\int_a^b f(x)\,dx \approx \frac{h}{2}\left[f(a) + 2\sum_{i=1}^{n-1} f(x_i) + f(b)\right]$$

where $h = \frac{b-a}{n}$ is the width of each subinterval and $x_i = a + ih$ for $i = 1,2,\dots,n-1$



Trapezoidal Rule

Using the Taylor series expansion of $f(x)$ around x_i:

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

Integrating term-by-term over $[x_i, x_{i+1}]$:

$$\int_{x_i}^{x_{i+1}} f(x)\,dx = \int_{x_i}^{x_{i+1}} \left(f(x_i) + f'(x_i)(x - x_i) + \frac{f''(x_i)}{2!}(x - x_i)^2 + \frac{f'''(x_i)}{3!}(x - x_i)^3 + O\big((x - x_i)^4\big) \right) dx$$

For the first term $\int_{x_i}^{x_{i+1}} f(x_i)dx = f(x_i)(x_{i+1} - x_i) = f(x_i)h$ Here, $h = x_{i+1} - x_i$

For the second term $\int_{x_i}^{x_{i+1}} f'(x_i)(x - x_i)\,dx = \frac{f'(x_i)}{2}(x_{i+1} - x_i)^2 = \frac{f'(x_i)}{2}h^2$

Trapezoidal Rule

Using the previous slide, we can show that

$$\boxed{\int_{x_i}^{x_{i+1}} f(x)\,dx = hf(x_i) + \frac{h^2}{2} f'(x_i) + \frac{h^3}{6} f''(x_i) + O(h^4)}$$

Equation A

This is the correct expression for the integration.

Using the Taylor series, we also can derive an expression for $f(x_{i+1})$

$$f(x_{i+1}) = f(x_i) + f'(x_i)(x_{i+1} - x_i) + \frac{f''(x_i)}{2!}(x_{i+1} - x_i)^2 + \frac{f'''(x_i)}{3!}(x_{i+1} - x_i)^3 + O((x_{i+1} - x_i)^4)$$

Since, $h = x_{i+1} - x_i$

$$f(x_{i+1}) = f(x_i) + f'(a)h + \frac{f''(x_i)}{2!} h^2 + \frac{f'''(x_i)}{3!} h^3 + O(h^4)$$

Trapezoidal Rule

The trapezoidal approximation on the interval $[x_i, x_{i+1}]$ is:

$$\int_{x_i}^{x_{i+1}} f(x)\,dx = \frac{h}{2}[f(x_i) + f(x_{i+1})]$$

Using the previous expression, we can show that

$$\boxed{\frac{h}{2}\big(f(x_{i+1}) + f(x_i)\big) = \frac{h}{2}\left(f(x_i) + f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f'''(x_i)}{3!}h^3 + O(h^4)\right)}$$

Equation B

This is the approximated expression.

$$TE_i = hf(x_i) + \frac{h^2}{2}f'(x_i) + \frac{h^3}{6}f''(x_i) + O(h^4) - \frac{h}{2}\left(f(x_i) + f(x_i) + f'(a)h + \frac{f''(x_i)}{2!}h^2 + \frac{f'''(x_i)}{3!}h^3 + O(h^4)\right)$$

$$TE_i = \frac{h^3}{6}f''(x_i) + O(h^4) - \frac{f''(x_i)}{2!}\frac{h^3}{2} + \frac{f'''(x_i)}{3!}\frac{h^4}{2} + O(h^6) = -\frac{h^3}{12}f''(x_i) + \mathrm{O}(\mathrm{h}^4)$$

The truncation error of the trapezoidal rule for a **single interval** is proportional to h^3, i.e. it has the order of $O(h^3)$.

Trapezoidal Rule

Total truncation error is given by the sum of all the errors

$$TE = \sum_{i=1}^{n} TE_i$$

We can rewrite the truncation error as

$$TE = -\frac{h^3}{12}\sum_{i=1}^{n} f''(x_i)$$

If $f''(x)$'s average value is considered over $[a, b]$, we get:

$$f''(\varsigma) = \frac{1}{n}\sum_{i=1}^{n} f''(x_i)$$

We can rewrite the truncation error as

$$TE = -\frac{nh^3}{12}f''(\varsigma) = -\frac{(b-a)h^2}{12}f''(\varsigma)$$

The error in the Trapezoidal Rule is proportional to h^2.i .e. it has the order of $O(h^2)$.