

Lecture 1: Numerical Integration (I)

(Adapted from slides by Uriel Morzan)

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11. Oct. 2023

Numerical Integration - Introduction

Numerical integration is ...

- ... about calculating the numerical value of a definite Integral of some function $f(x)$, such as (in 1 dimension):

$$\int_a^b f(x) dx.$$

Numerical integration is not necessary if ...

- ... we know an analytical expression for $f(x)$ and a primitive $F(x) = \int f(x) dx$. Then

$$\int_a^b f(x) dx = F(b) - F(a).$$

For example:

$$\int_0^t x^2 \sin(x) dx = -2 + (2 - t^2) \cos(t) + 2t \sin(t).$$

Numerical Integration - Introduction

We need numerical integration because ...

- ... for many functions $f(x)$ the primitive function $F(x)$ is either
 - ▶ unknown, or
 - ▶ not “analytical” (i.e. expressible as an elementary function), such as $\int e^{-x^2} dx$.
- ... sometimes we don't even know an expression for $f(x)$, but it is itself the result of some numerical computation.

For example:

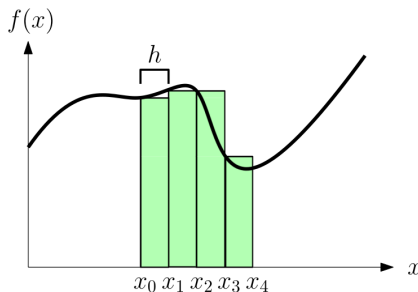
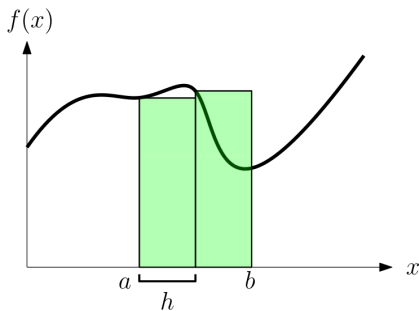
$$\int_{-\infty}^1 e^{-x^2} dx \simeq 1.63305$$

Numerical Integration Through the Integral Sum

Consider the definition of integrals via **the integral sum**:

$$\int_a^b f(x) \, dx \equiv \lim_{N \rightarrow \infty} \left[\sum_{k=0}^{N-1} f(x_k) \cdot h \right] \quad \text{with} \quad \begin{cases} h \equiv \frac{b-a}{N} \\ x_k \equiv a + k \cdot h \\ k = 0, \dots, N-1 \end{cases}$$

This is an approximation for finite N , but improves for growing N and is exact for $N \rightarrow \infty$.



Numerical Method: Left Riemann Sum

Define $I_L(N)$ as the approximated integral:

$$I_L(N) \equiv \sum_{k=0}^{N-1} f(x_k) \cdot h$$

with

$$h \equiv \frac{b-a}{N}$$

$$x_k \equiv a + k \cdot h$$

$$k = 0, \dots, N-1.$$

Algorithm: Left Riemann Sum

Input: function $f(x)$; boundaries a and b ; small threshold ϵ .

- ❶ Set N to some initial value, e.g. $N := 32$
- ❷ Compute $I_{\text{new}} := I_L(N)$
- ❸ Loop:
 - ▶ Increase N , e.g. $N := 2N$
 - ▶ Set $I_{\text{old}} := I_{\text{new}}$
 - ▶ Compute $I_{\text{new}} := I_L(N)$
 - ▶ If $|I_{\text{new}} - I_{\text{old}}| < \epsilon$ then exit the loop.

Output: I_{new} , which is an approximate value of $\int_a^b f(x) \, dx$

Numerical Method: Left Riemann Sum

Error scaling of the left Riemann sum

For large enough N the error decreases faster or as fast as $(1/N)^1$, i.e.

$$\int_a^b f(x) \, dx = I_L(N) + \mathcal{O}\left(\frac{1}{N}\right)$$

Assignment 7

Write a FORTRAN program that computes $\int_a^b f(x) dx$ for $f(x) = e^x$ using the left Riemann sum method:

- Write a function that takes the bounds a and b , and the desired precision ϵ .
- The function should integrate with the left Riemann sum, increasing N until the precision is achieved.
- The function should output the result at each step together with the current value for N .
- Test the function by calculating $\int_0^1 e^x dx$ with error threshold 10^{-5} in the main program and print the result.
- Submit your code as <surname>-assignment-7.f90 to gflux@ictp.it before the next lesson.

Hints:

- Create separate functions for $f(x)$ and the integration.
- Increase N significantly at each step (e.g., $N \leftarrow 2N$).
- No arrays are required.