

Introduction to Programming and Computational Physics

Lesson n.10

Numerical integration:

Trapezoidal rule

Simpson's rule

Definite Integrals

The evaluation of definite integral $\int_a^b f(x)dx$ is easily done if we know how to evaluate the antiderivative $F(x)$

then the solution will be then

$$\left[F(x) \right]_a^b = F(b) - F(a)$$

(It is the Fundamental Theorem of Calculus)

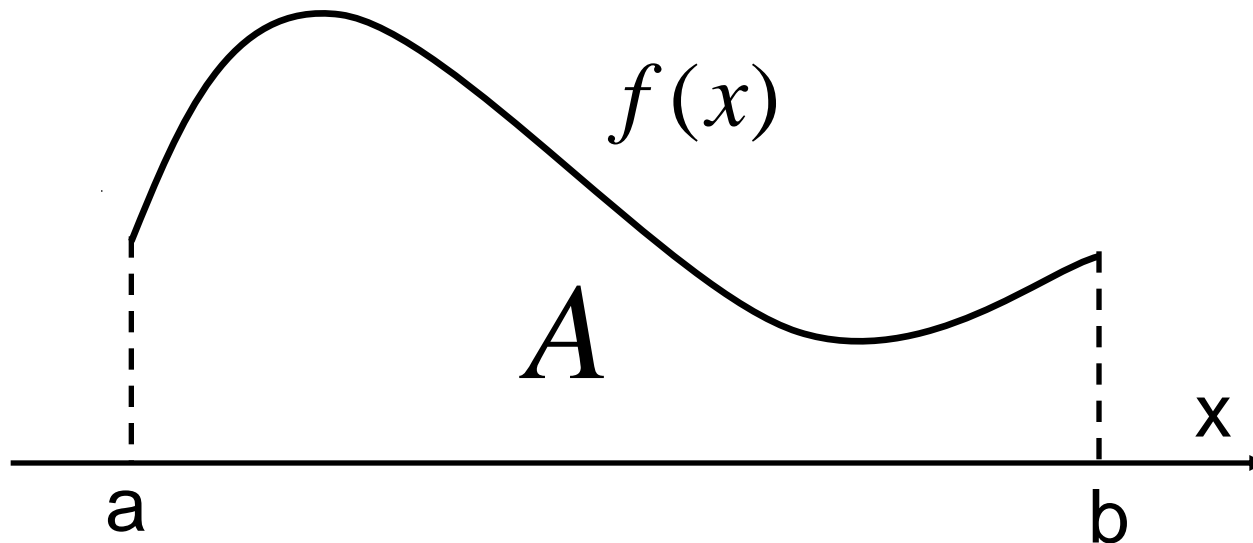
What we do when we can't calculate the antiderivative? How to evaluate for instance

$$\int_0^2 e^{-x^2} dx$$

Let's start with the geometrical interpretation of a definite integral

$$\int_a^b f(x) dx = A$$

as the area of the region under the curve



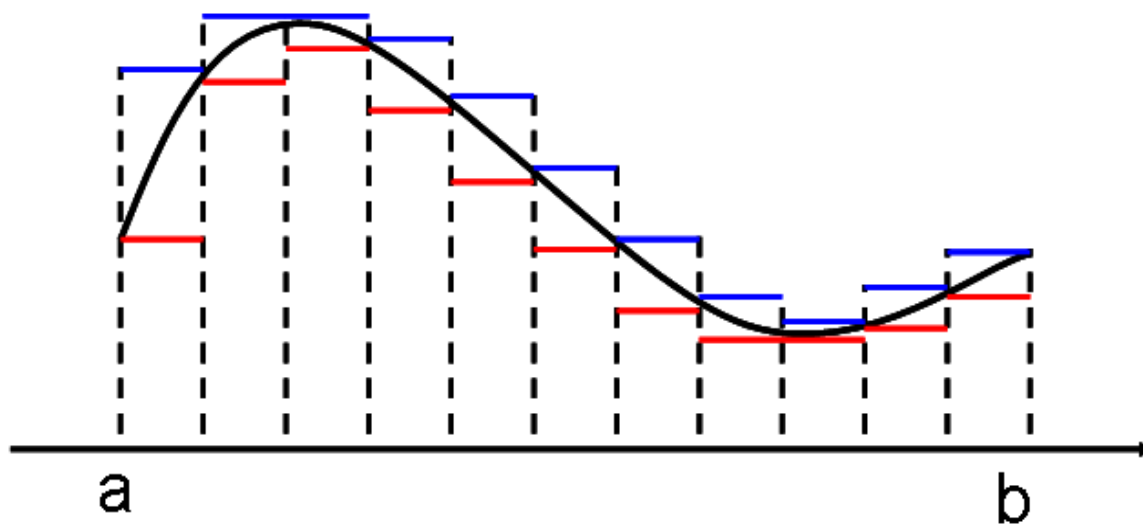
Riemann-Integral

Given a *limited* function $f : [a, b] \rightarrow \mathbb{R}$ $-M < f(x) < M$

$$S = \{x_0, x_1, \dots, x_n\} \quad \text{with} \quad a = x_0 < x_1 < \dots < x_n = b$$

Riemann *lower* and *upper* sums:

$$\Sigma'(f, S) = \sum_{i=0}^n \left[\inf_{x \in [x_j, x_{j+1}]} f(x) \right] (x_{j+1} - x_j) \quad \Sigma''(f, S) = \sum_{i=0}^n \left[\sup_{x \in [x_j, x_{j+1}]} f(x) \right] (x_{j+1} - x_j)$$



lower and upper integrals:

$$I'(f) = \sup_S \Sigma'(f, S) \qquad I''(f) = \inf_S \Sigma''(f, S)$$

(evaluated for all the possible partitions S)

with $I'(f) \leq I''(f)$

If $I'(f) = I''(f)$ the function is *Riemann-integrable*

Rectangular rule

Given $S = \{x_0, x_1, \dots, x_n\}$ Riemann *lower* and *upper* sums would constitute an **approximation** of the integral.

Anyway $\inf f(x)$ and $\sup f(x)$ over each interval are not easy to evaluate. We can consider instead the values of the function at the mid-point of each interval.

$$\int_a^b f(x) dx \sim \frac{(b-a)}{n} \sum_{i=0}^{n-1} f\left(a + \left(\frac{b-a}{n}\right)\left(i + \frac{1}{2}\right)\right)$$

This is the so-called **rectangular rule**.

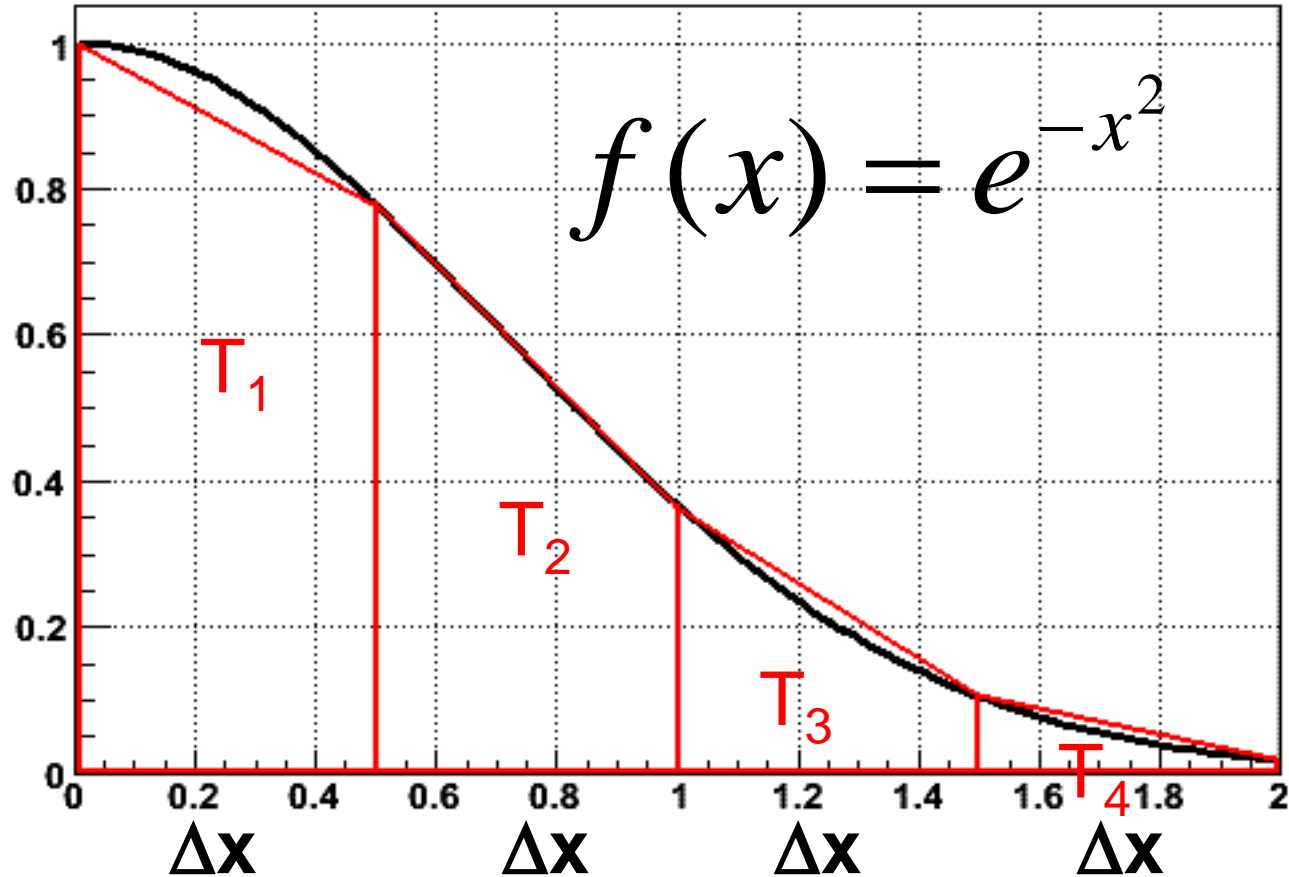
Numerical integration

In general, numerical integration will always be a sum:

$$\int_a^b f(x)dx \sim \sum_{i=0}^n c_i f(x_i) \quad x_i \in [a, b] \quad f(x_i)$$

Our aim is that our approximation is as accurate as possible with the minimum number of calculations of the function

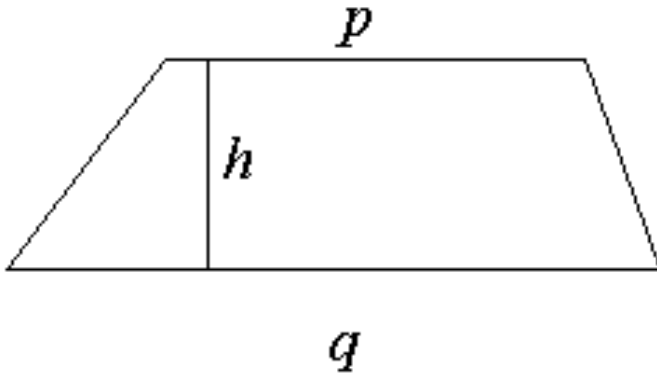
The trapezoidal rule



We divide the interval in N parts (here 4) and then

$$\int_0^2 e^{-x^2} dx \approx T_1 + T_2 + T_3 + T_4$$

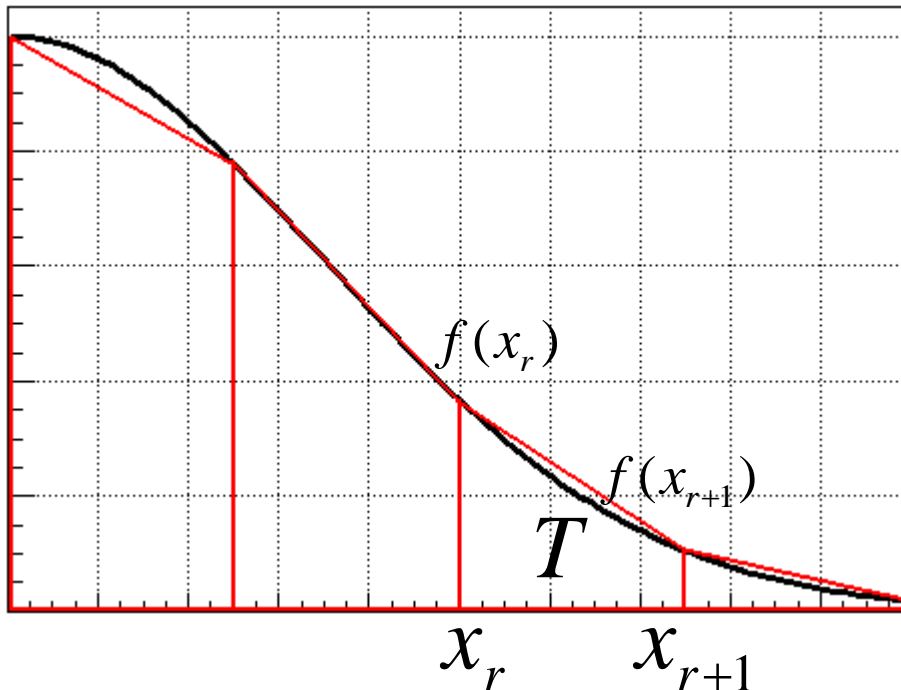
The area of a trapezoid is given by:



$$Area = \frac{h}{2} (p + q)$$

Our trapezoids are rotated 90 degrees, so that $h = \Delta x$ and

$$T = \frac{\Delta x}{2} (f(x_r) + f(x_{r+1}))$$



$$\Delta x = (x_{r+1} - x_r)$$

given $S = \{x_0, x_1, \dots, x_n\}$ $a = x_0 < x_1 < \dots < x_n = b$

An approximation of the integral is given by the application of the trapezoidal rule to the whole set

$$I \approx \frac{\Delta x}{2} (f_0 + f_1) + \frac{\Delta x}{2} (f_1 + f_2) + \dots + \frac{\Delta x}{2} (f_{n-2} + f_{n-1}) + \frac{\Delta x}{2} (f_{n-1} + f_n)$$

$$I \approx \Delta x \left(\frac{1}{2} f_0 + f_1 + f_2 + \dots + f_{n-2} + f_{n-1} + \frac{1}{2} f_n \right)$$

This is the formula to be used for the trapezoidal rule

Implementation

Given a required precision ε we will have to refine more and more until we reach the desired precision. The condition to be fulfilled is

$$|I_i - I_{i-1}| < \varepsilon |I_{i-1}|$$

We can move from $S = \{x_0, x_1, \dots, x_n\}$ to the new sample

$S' = \{x_0, x_1, \dots, x_{2n}\}$ just adding the middle point between each point of the previous sample

Code optimization...

In order to avoid the re-evaluation of the function at the same abscissa the following algorithm could be used

$$c = b - a$$

$$J_1 = \frac{1}{2} (f(a) + f(b))$$

$$I_1 = cJ_1$$

$$J_2 = J_1 + f(a + \frac{1}{2}c)$$

$$I_2 = \frac{1}{2}cJ_2$$

$$J_4 = J_2 + f(a + \frac{1}{4}c) + f(a + \frac{3}{4}c)$$

$$I_4 = \frac{1}{4}cJ_4$$

$$J_8 = J_4 + f(a + \frac{1}{8}c) + f(a + \frac{3}{8}c) + f(a + \frac{5}{8}c) + f(a + \frac{7}{8}c)$$

$$I_8 = \frac{1}{8}cJ_8$$

As usual... first implement the easiest way and then try to improve it...

The error in the trapezoidal rule:

Taylor expansion: $f(x_r + t) = a_0 + a_1 t + a_2 t^2 + a_3 t^3 + \dots$

where: $a_m = \frac{1}{m!} f^{(m)}(x_r) = \frac{1}{m!} f_r^{(m)}$

Nb:

$$t = x - x_r = x - a - rh$$

$$\begin{aligned} \int_{x_r}^{x_{r+1}} f(x) dx &= \int_0^h f(x_r + t) dt = \\ &= \left[a_0 t + \frac{1}{2} a_1 t^2 + \frac{1}{3} a_2 t^3 + \dots \right]_0^h = \\ &= a_0 h + \frac{1}{2} a_1 h^2 + \frac{1}{3} a_2 h^3 + \dots \end{aligned}$$

a)

From trapezoidal rule we have:

$$\begin{aligned} \int_{x_r}^{x_{r+1}} f(x) dx &\approx \frac{1}{2} h (f_r + f_{r+1}) = & \text{Nb: } f_r &= a_0 \\ &= \frac{1}{2} h \{ (a_0) + (a_0 + a_1 h + a_2 h^2 + \dots) \} = & f_{r+1} &= f(x_r + h) \\ &= a_0 h + \frac{1}{2} a_1 h^2 + \frac{1}{2} a_2 h^3 + \dots & & \text{b)} \end{aligned}$$

If we compare a) and b) and neglect terms $O(h^4)$

the error for one strip will be $\frac{1}{6} a_2 h^3 = \frac{1}{12} h^3 f_r''$

and for n strips $\frac{1}{12} n h^3 \overline{f''}$

$\overline{f''}$ is f'' evaluated in a given value in $[a, b]$

but
$$h = \frac{(b-a)}{n}$$

the error becomes
$$\frac{1}{12} h^2 (b-a) \overline{f''}$$

or
$$\frac{1}{12} \frac{(b-a)^3}{n^2} \overline{f''}$$

and we will say that for the trapezoidal rule the error is $\sim h^2$ or $\sim 1/n^2$

Newton-Cotes formulas

They are a group of formulas for numerical integration based on evaluating the integrand at equally-spaced points. Given a partition $a = x_0 < x_1 < \dots < x_n = b$ if the values $f(a)$, $f(b)$ are used we will refer to a *closed* formula, otherwise to an *open* formula.

The rectangular rule is an open formula:

$$\int_a^b f(x)dx \sim \frac{(b-a)}{n} \sum_{i=0}^{n-1} f\left(a + \left(\frac{b-a}{n}\right)\left(i + \frac{1}{2}\right)\right)$$

The trapezoidal rule is a closed formula:

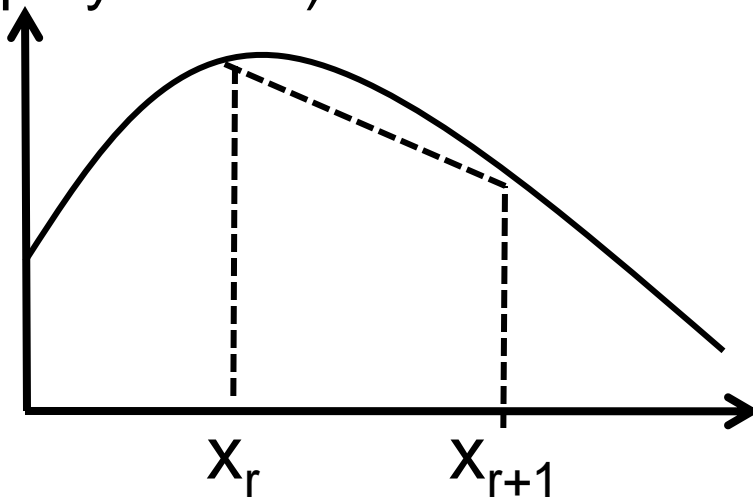
$$\int_a^b f(x)dx \sim \frac{(b-a)}{n} \left(\frac{1}{2} (f(a) + f(b)) + \sum_{i=1}^{n-1} f\left(a + i\left(\frac{b-a}{n}\right)\right) \right)$$

Newton-Cotes formulas

Given a partition $a = x_0 < x_1 < \dots < x_n = b$ and a set of n points

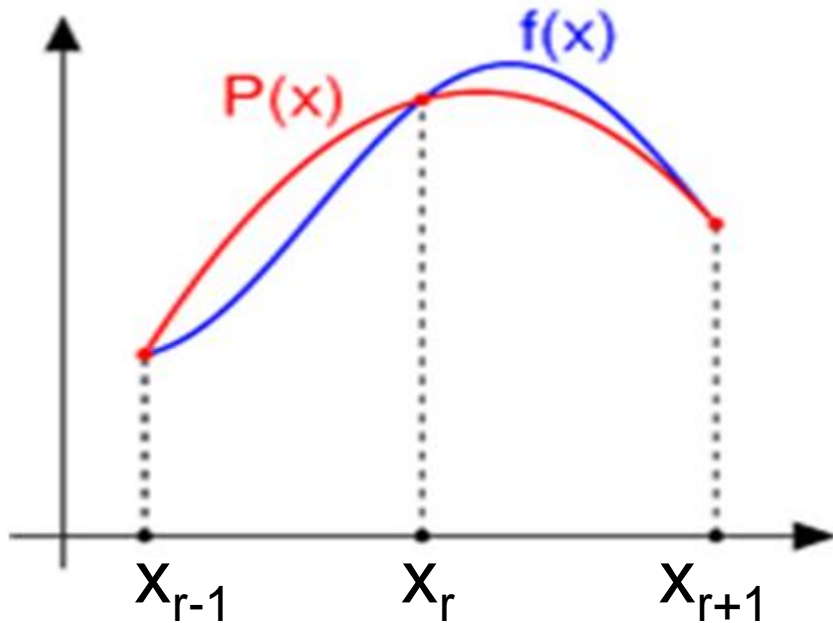
$$((x_0, f(x_0)), (x_1, f(x_1)), \dots, (x_n, f(x_n)))$$

it is always possible to find an $n-1$ degree polynomial passing through the n points (Lagrange interpolating polynomial)



Trapezoidal rule:
2 points, 1-degree polynomial interpolation
(linear interpolation)

The Simpson's rule:



Simpson's rule can be derived by approximating the integrand $f(x)$ by the quadratic interpolant $P(x)$

3 points, 2-degree polynomial interpolation
(quadratic interpolation)

This means that given a partition $S = \{a = x_0 < x_1 < \dots < x_n = b\}$ the evaluation of the integral can be obtained by applying n times the trapezoidal rule or $n/2$ times the Simpson rule

The Simpson's rule:

The formula to be used for the Simpson rule is

$$\int_{x_{r-1}}^{x_{r+1}} f(x)dx \sim \frac{1}{3} h(f_{r-1} + 4f_r + f_{r+1})$$

If we divide $[a,b]$ in n intervals (n even)

$$\begin{aligned} \int_a^b f(x)dx &\sim \frac{1}{3} h \{ (f_0 + 4f_1 + f_2) + (f_2 + 4f_3 + f_4) + \dots + (f_{n-2} + 4f_{n-1} + f_n) \} = \\ &= \frac{1}{3} h (f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + \dots + 2f_{n-2} + 4f_{n-1} + f_n) \end{aligned}$$

The error in the Simpson's rule:

For a given 2-strips the error is $\frac{1}{90} h^5 f_r^{iv}$

For $n/2$ 2-strips the error is

$$\frac{1}{90} \frac{n}{2} h^5 \overline{f^{iv}} = \frac{1}{180} (b-a) h^4 \overline{f^{iv}} = \frac{1}{180} \frac{(b-a)^5}{n^4} \overline{f^{iv}}$$

and we will say that for the Simpson's rule the error is $\sim h^4$ or $\sim 1/n^4$ (it was $\sim 1/n^2$ for the trapezoidal rule)