Introduction to Programming and Computational Physics

Lecture 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)

In this case, the solution will be

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

(Fundamental Theorem of Calculus)

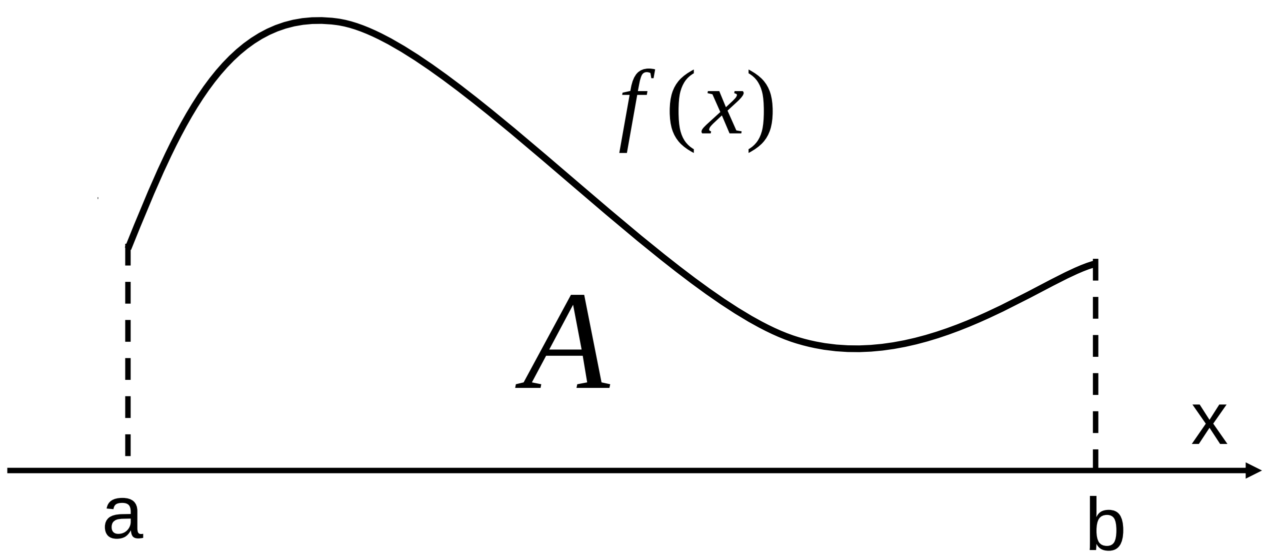
What if we can't calculate the antiderivative? How to evaluate for instance

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

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



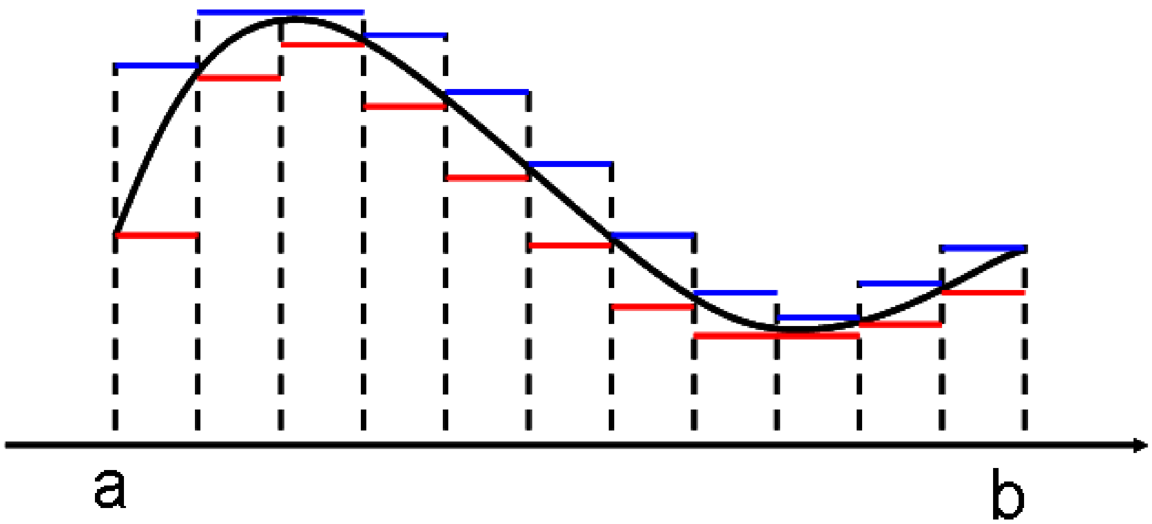
Riemann-Integral

Given a *limited* function $f:[a,b] \to R \qquad -M < f(x) < M$

$S = \{x_0, x_1, ..., x_n\}$ with $a = x_0 < x_1 < ... < x_n = b$

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 $S = \{x_0, x_1, ..., x_n\}$ 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.

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

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

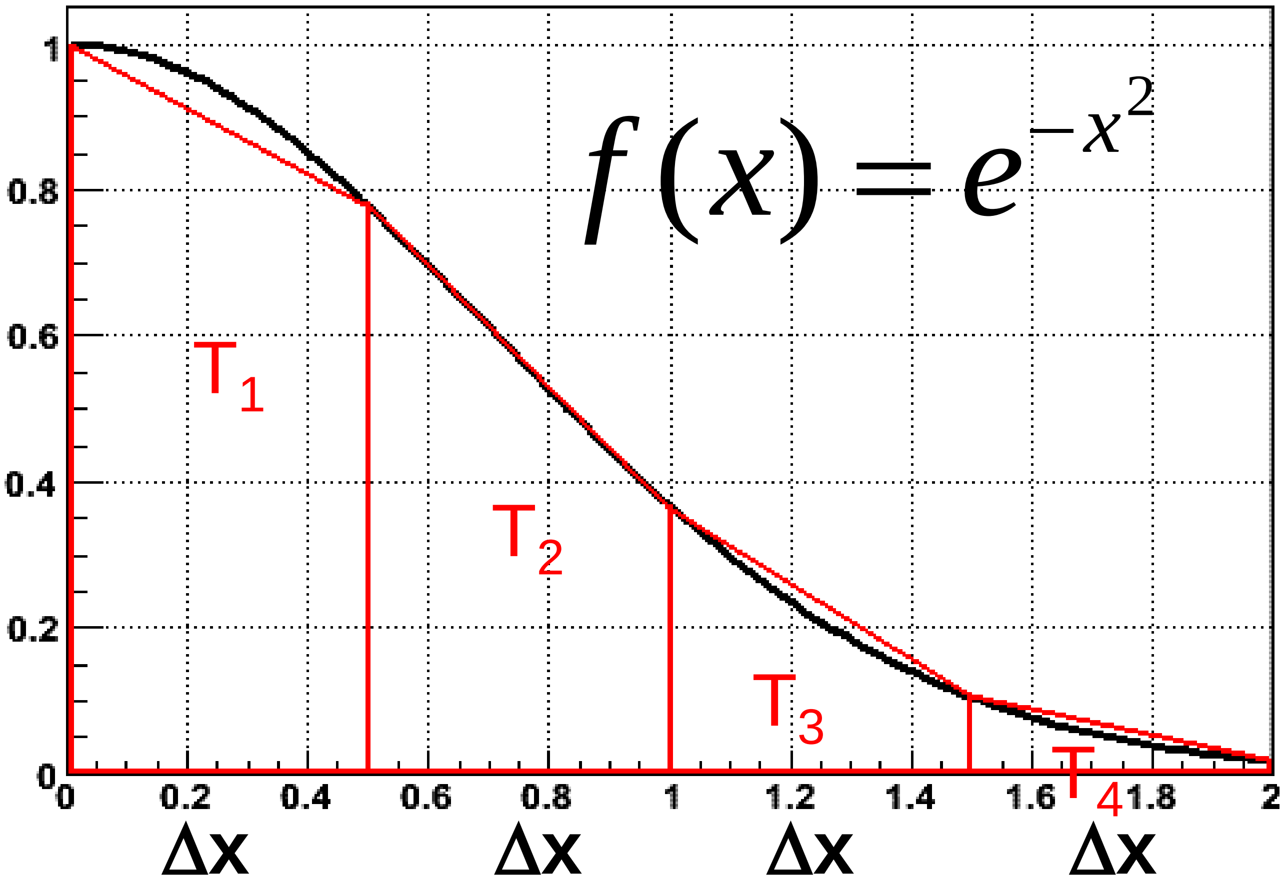
Numerical integration

In general, numerical integration will always be a sum:

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

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

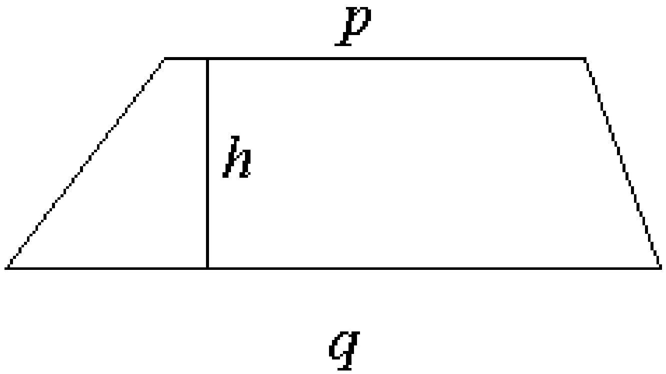
The trapezoidal rule



We subdivide the interval (0,2) 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:

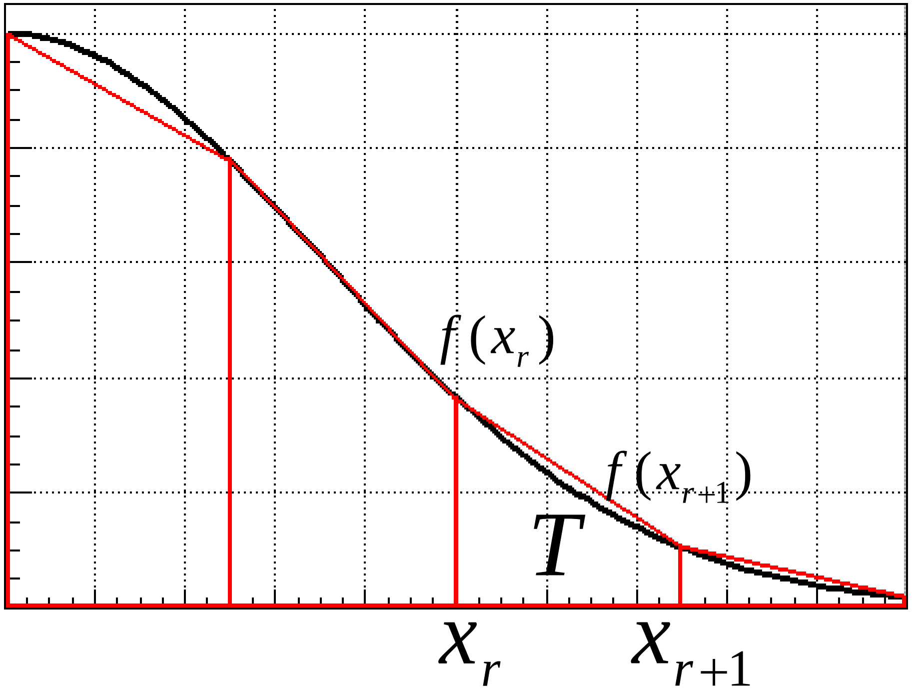


$$Area = \frac{h}{2}(p+q)$$

Our trapezoids are rotated 90 degrees, so that h = Δx and

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

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



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

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

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

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

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 (relative precision)

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

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

$S' = \{x_0, x_1, ..., x_{2n}\}$ 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

$$c = b - a$$

$$J_1 = \tfrac{1}{2}(f(a) + f(b)) \qquad I_1 = cJ_1$$

$$J_2 = J_1 + f(a + \tfrac{1}{2}c) \qquad I_2 = \tfrac{1}{2}cJ_2$$

$$J_4 = J_2 + f(a + \tfrac{1}{4}c) + f(a + \tfrac{3}{4}c) \qquad I_4 = \tfrac{1}{4}cJ_4$$

$$J_8 = J_4 + f(a + \tfrac{1}{8}c) + f(a + \tfrac{3}{8}c) + f(a + \tfrac{5}{8}c) + f(a + \tfrac{7}{8}c) \qquad I_8 = \tfrac{1}{8}cJ_8$$

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

The error in the trapezoidal rule:

Taylor expansion: $$f(x_r+t)=a_0+a_1t+a_2t^2+a_3t^3+\dots$$

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

Nb:

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

$$\int_{x_r}^{x_{r+1}}f(x)dx=\int_0^h f(x_r+t)dt=$$

$$=\left[a_0t+\tfrac{1}{2}a_1t^2+\tfrac{1}{3}a_2t^3+\dots\right]_0^h=$$

$$=a_0h+\tfrac{1}{2}a_1h^2+\tfrac{1}{3}a_2h^3+\dots$$ a)

From trapezoidal rule we have:

Nb: $f_r = a_0$

$f_{r+1} = f(x_r + h)$

$$\int_{x_r}^{x_{r+1}} f(x)dx \approx \tfrac{1}{2}h\left(f_r + f_{r+1}\right) =$$

$$= \tfrac{1}{2}h\left\{(a_0) + (a_0 + a_1 h + a_2 h^2 + \ldots)\right\} =$$

$$= a_0 h + \tfrac{1}{2}a_1 h^2 + \tfrac{1}{2}a_2 h^3 + \ldots \qquad \text{b)}$$

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 $\frac{1}{12}nh^3\overline{f''}$

$\overline{f''}$ is f'' evaluated in an (unknown) value in [a,b] but $h = \dfrac{(b-a)}{n}$

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

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

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 $a = x_0 < x_1 < ... < x_n = b$ 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:

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

The trapezoidal rule is a closed formula:

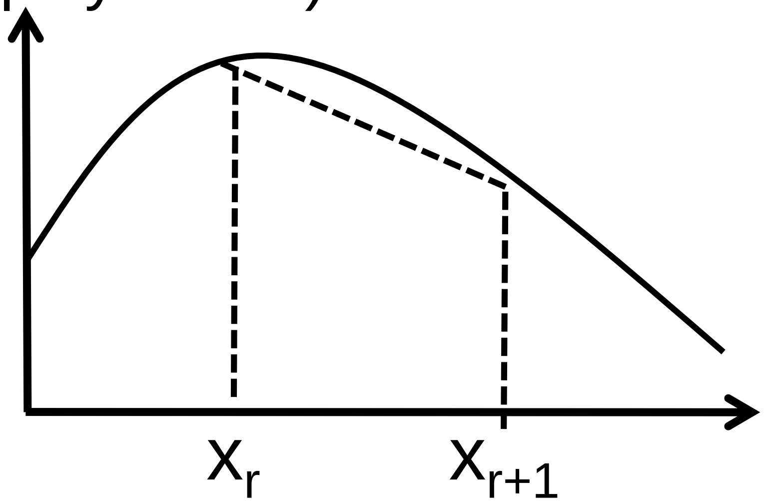
$$\int_a^b f(x)dx \sim \frac{(b-a)}{n}\left(\tfrac{1}{2}(f(a)+f(b))+\sum_{i=1}^{n-1} f(a+i(\tfrac{b-a}{n}))\right)$$

Newton-Cotes formulas

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

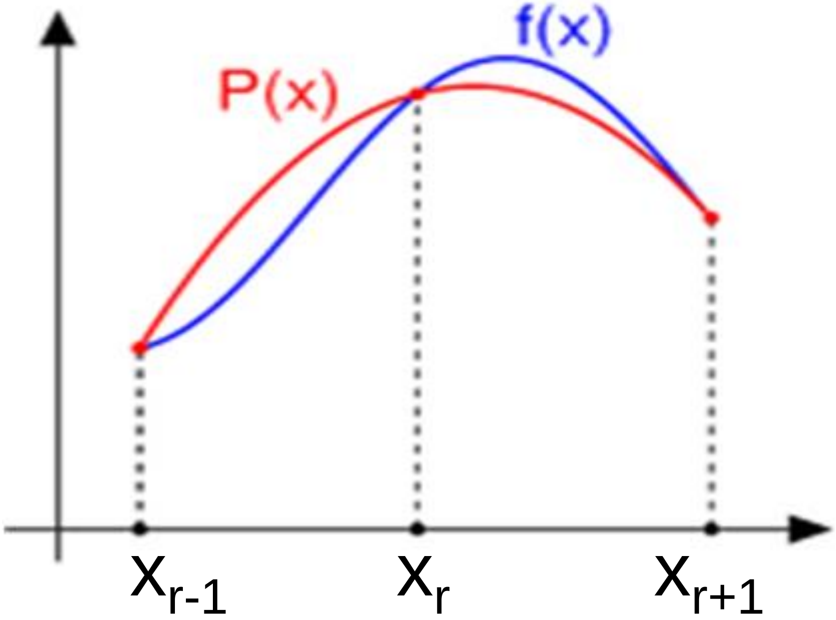
$$((x_0, f(x_0)), (x_1, f(x_1)), ..., (x_n, f(x_n)))$$

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 $S = \{a = x_0 < x_1 < ... < x_n = b\}$ 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

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

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

$$\int_a^b f(x)dx \sim \tfrac{1}{3}h\{(f_0 + 4f_1 + f_2) + (f_2 + 4f_3 + f_4) + ... + (f_{n-2} + 4f_{n-1} + f_n)\} =$$

$$= \tfrac{1}{3}h\left(f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + ... + 2f_{n-2} + 4f_{n-1} + f_n\right)$$

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 ~h^4 or ~$1/n^4$ (it was ~$1/n^2$ for the trapezoidal rule)