Chapter III: Numerical Integration

In this chapter, we will study some approximate methods for calculating definite integrals. These methods also allow the calculation of integrals that do not have direct or analytical solutions. We can also calculate the integral of a function given in tabular or discrete form.

3.1 Trapezoidal Rule

This formula is very simple; it allows us to replace the curve ***f(x)*** of the function to be integrated by a straight line that connects the points ***(a, f(a))*** and ***(b, f(b))***, which gives a trapezoid (Fig. 3.1).

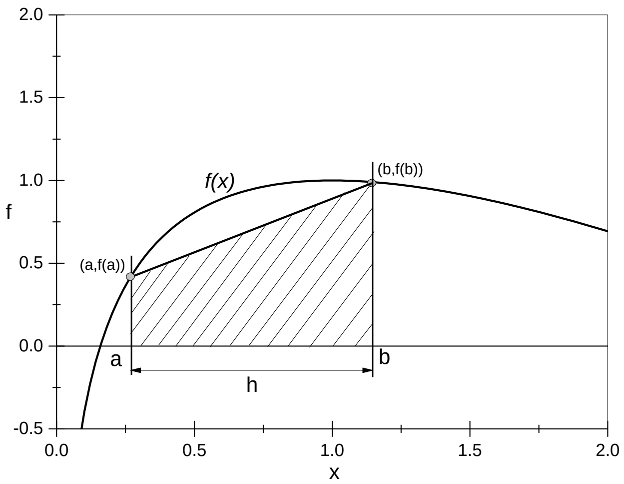

Fig. 3.1: Trapezoidal Method

The integral is thus replaced by the area of the trapezoid:

$$\boldsymbol{s = \int_a^b f(x) = \frac{h}{2}(f(a) + f(b))}$$

With ***h = b-a*** is called the integration step. We can notice that there is a significant difference between the curve of the function and the straight line, which means that we make a calculation error. To minimize this error, we use another more suitable form of this formula.

3.1.1 Generalized Trapezoidal Rule

We divide the interval ***[a, b]*** into several equal subintervals and apply the trapezoidal rule to each subinterval (Fig. 3.2). We thus have the subintervals $[\boldsymbol{a = x_0, x_1}] \cup [\boldsymbol{x_1, x_2}] \cup \ldots\ldots \cup [\boldsymbol{x_{n-1}, x_n = b}]$, the application of the trapezoidal rule gives:

$$\int_a^b f(x) = \frac{h}{2}(f(x_0) + f(x_1)) + \frac{h}{2}(f(x_1) + f(x_2)) + \frac{h}{2}(f(x_2) + f(x_3)) + \cdots + \frac{h}{2}(f(x_{n-1}) + f(x_n))$$

$$\int_a^b f(x) = \frac{h}{2}\left(f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)\right) = \frac{h}{2}\left(f_0 + 2\sum_{i=1}^{n-1} f_i + f_n\right)$$

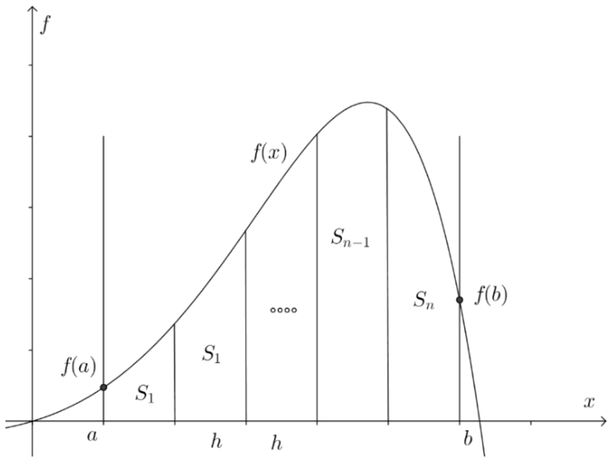

Fig. 3.2: Generalized Trapezoidal Method

3.1.2 Integration Error

This is the difference between the exact integral of the function and that calculated by the trapezoidal method; it is denoted by ***R(f).***

$$\boldsymbol{R(f) = \int_{x_0}^{x_n} f(x)dx - \frac{h}{2}\left(f_0 + 2\sum_{i=1}^{n-1} f_i + f_n\right) = -\frac{b-a}{12}h^2 f''(z)} \quad \text{with} \quad \boldsymbol{z \in [a, b]}$$

Example: Let's calculate the integral $\int_0^1 e^{-x^2}dx$ with an accuracy of 0.001 by the trapezoidal method. We must first find the number of divisions to make to obtain this accuracy. The integration error is written $\boldsymbol{R(f) = -\frac{b-a}{12}h^2 f''(z)}$ as its absolute value must be less than or equal to the given accuracy (0.001), i.e.:

$$|\boldsymbol{R(f)}| = \left|-\frac{\boldsymbol{b-a}}{\boldsymbol{12}}\boldsymbol{h^2 f''(z)}\right| \leq \boldsymbol{0.001}$$

The function $f(x) = e^{-x^2}$, so its second derivative is $f''(x) = 2(2x^2 - 1)e^{-x^2}$, this function is strictly increasing in the given interval (Fig. 3.3).

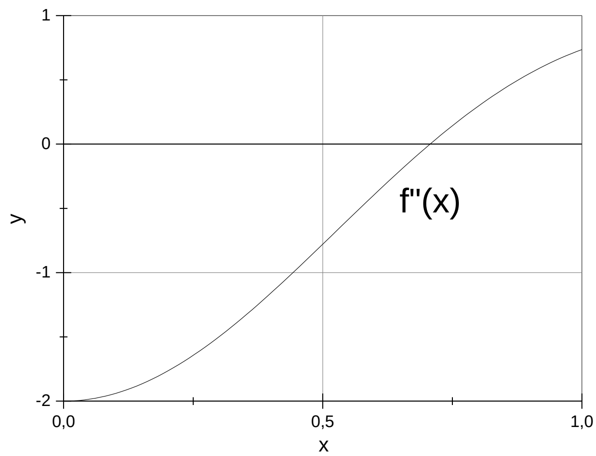

Fig. 3.3. Second derivative curve of e^{-x^2}

We calculate $M = max|\boldsymbol{f''(z)}| = \boldsymbol{2}$ à $\boldsymbol{x = 0}$

So $|\boldsymbol{R(f)}| = \left|-\frac{\boldsymbol{b-a}}{\boldsymbol{12}}\boldsymbol{h^2 f''(z)}\right| \leq \boldsymbol{0.001}$

Hence $\boldsymbol{h} \leq \sqrt{\frac{\mathbf{12*0.001}}{\mathbf{(1-0)*2}}} = \mathbf{0.0774}$ then $\mathrm{n} = \frac{\mathbf{1}}{\mathbf{0.0774}} = \mathbf{12.91}$ we have 13 divisions.

The integration step $h = \frac{1}{13}$.

$$\int_0^1 e^{-x^2} dx = \frac{1}{2*13}\left(e^{-0^2} + 2\sum_{i=1}^{12} e^{-(\frac{i}{13})^2} + e^{-1^2}\right) = 0.74646$$

3.2 Simpson's Rules

In this formula, we do not replace the function with a straight line but with a parabola of degree ***n*** less than or equal to two. The latter must pass through three points $(\boldsymbol{x_0}, \boldsymbol{y_0}), (\boldsymbol{x_1}, \boldsymbol{y_1})\mathbf{et}\ (\boldsymbol{x_2}, \boldsymbol{y_2})$, which means that this method is only applicable for an even number of slices (a slice is the interval between two points) (Fig. 3.4.). Simpson's formula is written:

$$\int_{\boldsymbol{a}}^{\boldsymbol{b}} \boldsymbol{f}(\boldsymbol{x}) \cong \frac{\boldsymbol{h}}{\mathbf{3}}\left(\boldsymbol{f}(\boldsymbol{x_0}) + \mathbf{4}\boldsymbol{f}(\boldsymbol{x_1}) + \boldsymbol{f}(\boldsymbol{x_2})\right)$$

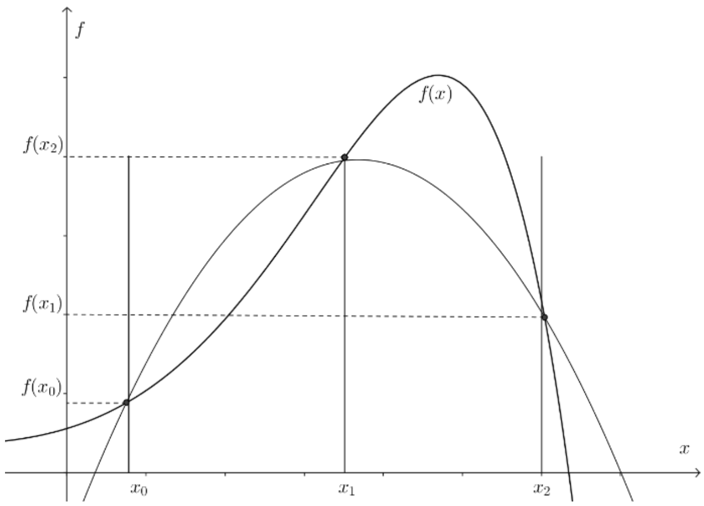

Fig. 3.4: Simpson's Method

If we generalize Simpson's formula for ***2n*** subintervals with an integration step $\boldsymbol{h} = \frac{\boldsymbol{b}-\boldsymbol{a}}{\boldsymbol{2n}}$, $\boldsymbol{a} = \boldsymbol{x_0} < \boldsymbol{x_1} < \cdots \ldots . < \boldsymbol{x_{2n}} = \boldsymbol{b}$ and $\boldsymbol{x_k} = \boldsymbol{a} + \boldsymbol{hk}$, for k=0,1,2,......,2n.

The generalized Simpson's formula is written:

$$\int_{\boldsymbol{a}}^{\boldsymbol{b}} \boldsymbol{f}(\boldsymbol{x}) \cong \frac{\boldsymbol{h}}{\mathbf{3}}\left(\boldsymbol{f}(\boldsymbol{x_0}) + \mathbf{2}\sum\nolimits_{\boldsymbol{i}\ \boldsymbol{pair}} \boldsymbol{f}(\boldsymbol{x_i}) + \mathbf{4}\sum\nolimits_{\boldsymbol{i}\ \boldsymbol{impair}} \boldsymbol{f}(\boldsymbol{x_i}) + \boldsymbol{f}(\boldsymbol{x_{2n}})\right)$$

The interpolation error of Simpson's formula is written:

$$\boldsymbol{R}(\boldsymbol{f}) = -\frac{\boldsymbol{b}-\boldsymbol{a}}{\mathbf{180}}\boldsymbol{h}^{\mathbf{4}}\boldsymbol{f}^{(\mathbf{4})}(\boldsymbol{z}) \text{ with } \boldsymbol{z} \in [\boldsymbol{a}, \boldsymbol{b}]$$

Example: Let's calculate the integral $\int_0^1 e^{-x^2} dx$ with an accuracy of ***0.001*** by Simpson's method. We must first find the number of divisions to make to obtain this accuracy.

The integration error is written: $\boldsymbol{R}(\boldsymbol{f}) = -\frac{(\boldsymbol{b}-\boldsymbol{a})}{\mathbf{180}}\boldsymbol{h}^{\mathbf{4}}\boldsymbol{f}^{(\mathbf{4})}(\boldsymbol{z})$

its absolute value must be less than or equal to the given accuracy (0.001), i.e.:

$$|\boldsymbol{R}(\boldsymbol{f})| = \left|-\frac{(\boldsymbol{b}-\boldsymbol{a})}{\mathbf{180}}\boldsymbol{h}^4\boldsymbol{f}^{(4)}(\boldsymbol{z})\right| \leq \mathbf{0.001}$$

The function is $f(x) = e^{-x^2}$, its fourth derivative $f^{(4)}(x) = (16x^4 - 48x^2 + 12)e^{-x^2}$, this function is not monotonic in the given interval. We calculate its maximum by the Origin plotter (Fig. 3.5.).

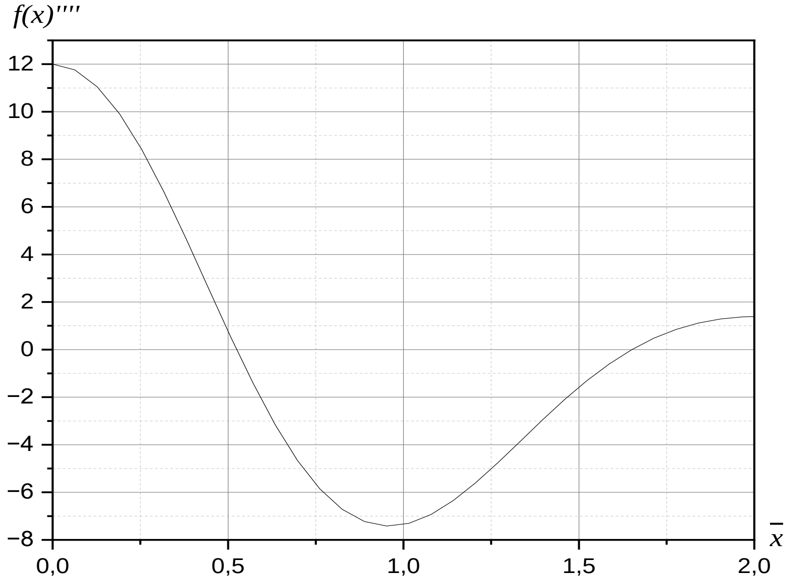

Fig. 3.5. Fourth derivative curve of e^{-x^2}

$M = max\left|\boldsymbol{f}^{(4)}(\boldsymbol{z})\right| = \mathbf{12}$ à $\boldsymbol{x} = \mathbf{0}$. We have $\boldsymbol{h} \leq \sqrt[4]{\frac{\mathbf{180*0.001}}{\mathbf{(1-0)*12}}} = \mathbf{0.35}$ then $\mathbf{2}\boldsymbol{n} = \frac{\mathbf{1}}{\mathbf{0.35}} = \mathbf{2.85}$ **so** ***2n=4*.** And the integration step $h = \frac{1}{4} = 0.25$.

We find: $\int_0^1 e^{-x^2}dx = \frac{0.25}{3}\left(e^{-0^2} + 4(e^{-0.25^2} + e^{-0.75^2}) + 2e^{-0.5^2} + e^{-1^2}\right) = 0.7469$

3.3 Quadrature Method

This method allows the development of numerical integration formulas based on the Lagrange polynomial. For example, the trapezoidal and Simpson's rules can be found using this method, or other more efficient integration formulas can be constructed. In this method, the function is replaced by a Lagrange polynomial, then the found polynomial is integrated. We can write:

$$\boldsymbol{f}(\boldsymbol{x}) \cong \boldsymbol{P}_{\boldsymbol{n}}(\boldsymbol{x}) = \sum_{\boldsymbol{i}=\mathbf{0}}^{\boldsymbol{n}} \boldsymbol{f}_{\boldsymbol{i}}\boldsymbol{L}_{\boldsymbol{i}}(\boldsymbol{x})$$

where ***P(x)*** is the Lagrange polynomial approximating ***f(x)***.

Integrating:

$$\int_{\boldsymbol{a}}^{\boldsymbol{b}} \boldsymbol{f}(\boldsymbol{x})\boldsymbol{dx} \cong \int_{\boldsymbol{a}}^{\boldsymbol{b}} \boldsymbol{P}_{\boldsymbol{n}}(\boldsymbol{x})\boldsymbol{dx} = \sum_{\boldsymbol{i}=\mathbf{0}}^{\boldsymbol{n}} \boldsymbol{f}_{\boldsymbol{i}} \int_{\boldsymbol{a}}^{\boldsymbol{b}} \boldsymbol{L}_{\boldsymbol{i}}(\boldsymbol{x})\boldsymbol{dx}$$

If we set:

$$\boldsymbol{A}_{\boldsymbol{i}} = \int_{\boldsymbol{a}}^{\boldsymbol{b}} \boldsymbol{L}_{\boldsymbol{i}}(\boldsymbol{x})\boldsymbol{dx} \ \text{ pour } \boldsymbol{i=0,1,\ldots,n}$$

where $L_i(x)$ are the Lagrange basis polynomials.

We obtain the quadrature formula:

$$\int_a^b f(x)dx \cong \sum_{i=0}^{n} f_i A_i$$

We must now choose the form of the function ***f(x)***. In our case, we take:

$$f(x) = x^k \quad \text{with} \quad k=0,1,2,\dots,n$$

Substituting into the integral:

$$\int_a^b x^k dx \cong \sum_{i=0}^{n} f_i A_i = \frac{b^{k+1}-a^{k+1}}{k+1} \quad k=0,1,2,\dots,n$$

By varying *i* from 0 to *n* for each value of *k*, we will have:

for k=0: $x_0^0 A_0 + x_1^0 A_1 + \cdots \dots + x_n^0 A_0 = \frac{b^1-a^1}{1}$

for k=1: $x_0^1 A_0 + x_1^1 A_1 + \cdots \dots + x_n^1 A_0 = \frac{b^2-a^2}{2}$

for k=2: $x_0^2 A_0 + x_1^2 A_1 + \cdots \dots + x_n^2 A_0 = \frac{b^3-a^3}{3}$

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for k=n: $x_0^n A_0 + x_1^n A_1 + \cdots \dots + x_n^n A_0 = \frac{b^{n+1}-a^{n+1}}{n+1}$

Thus, we obtain for all values of *i* and *k* the following system:

$$\begin{bmatrix} 1 & 1 & 1 & \dots\dots 1 \\ x_0 & x_1 & x_2 & \dots\dots x_n \\ x_0^2 & x_1^2 & x_2^2 & \dots . x_n^2 \\ \dots & \dots & \dots & \dots \\ x_0^n & x_1^n & x_2^n & \dots . x_n^n \end{bmatrix} \begin{bmatrix} A_0 \\ A_1 \\ A_2 \\ . \\ A_n \end{bmatrix} = \begin{bmatrix} I_0 \\ I_1 \\ I_2 \\ . \\ I_n \end{bmatrix} \quad \text{with} \quad I_k = \frac{b^{k+1}-a^{k+1}}{k+1}$$

The determinant of the matrix of the found system is called the "Von-Dermonde" determinant. It is non-zero, therefore the solution of this system exists and is unique $(A_0, A_1, \dots\dots, A_n)$.

Example:

Let's calculate the integral $\int_0^1 e^{-x^2} dx$ with a formula of the following form:

$$\int_0^1 e^{-x^2} dx = A_0 f(0) + A_1 f(0.25) + A_2 f(0.5) + A_3 f(0.75) + A_2 f(1.00)$$

In this case, we first look for the constants A_i, then we calculate the integral. These constants are given by the following system of equations:

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 0 & 0.25 & 0.5 & 0.75 & 1 \\ 0 & 0.0625 & 0.25 & 0.5626 & 1 \\ 0 & 0.015625 & 0.125 & 0.421875 & 1 \\ 0 & 0.00390625 & 0.0625 & 0.31640625 & 1 \end{bmatrix} \begin{bmatrix} A_0 \\ A_1 \\ A_2 \\ A_3 \\ A_4 \end{bmatrix} = \begin{bmatrix} 1 \\ 0.5 \\ 0.333 \\ 0.250 \\ 0.200 \end{bmatrix}$$

The solution of the system is (0.0691, 0.3812, 0.1052, 0.3694, 0.0751), therefore:

$$\int_0^1 e^{-x^2} dx = 0.0691 e^{0} + 0.3812 e^{-0.25^2} + 0.1052 e^{-0.5^2} + 0.3694 e^{-0.75^2} + 0.0751 e^{-1^2} = \mathbf{0.7472}$$

This is the quadrature formula for this specific example. You would then need to know the function *f(x)* and the values of x_0, x_1, x_2, x_3, and x_4 to compute the approximate value of the integral.