Chapter 3

Integration numerical

3.1 Introduction:

The calculation of limited integration of a function over a domain is equivalent to the calculation of the area delimited under the curve (fig. 3.1).

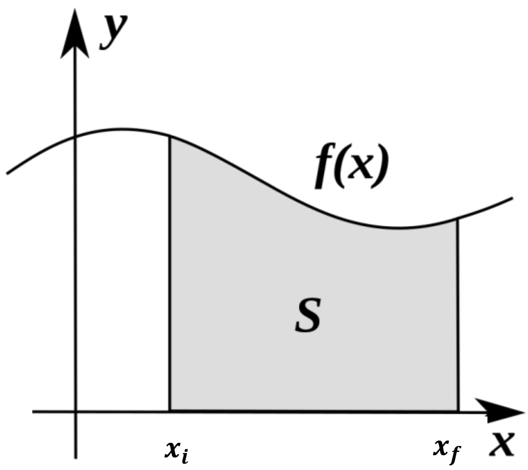

Figure 3.1 : Limited intégration of a fonction f(x)

In some cases, this integral can be calculated analytically. However, most often, we encounter one of the following situations:

- The analytical calculation is long and complicated.
- The integral has no analytical expression at all.
- The function f is only presented at discrete points, for example, if it results from a physical measurement.

In these cases, we use numerical analysis to arrive at an approximated value. The principle of numerical integration in evaluating integration is to calculate the area. Numerical integration is based on dividing the segment $[x_i, x_f]$ into n equal intervals and summing their areas.

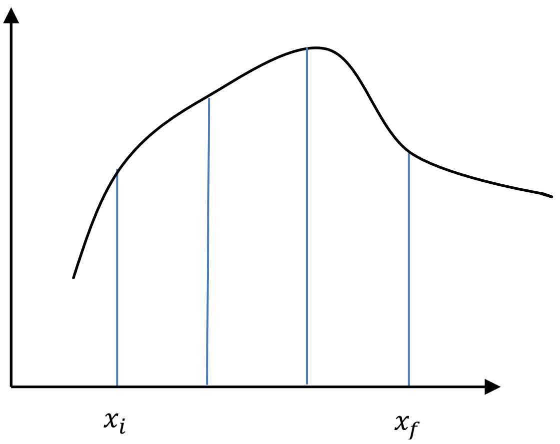

Figure 3.2: The principle of numerical integration

3. 2. Trapezoidal rule

The principle is to assimilate the area under the curve of the function to the area of a trapezoid (figure 3.3).

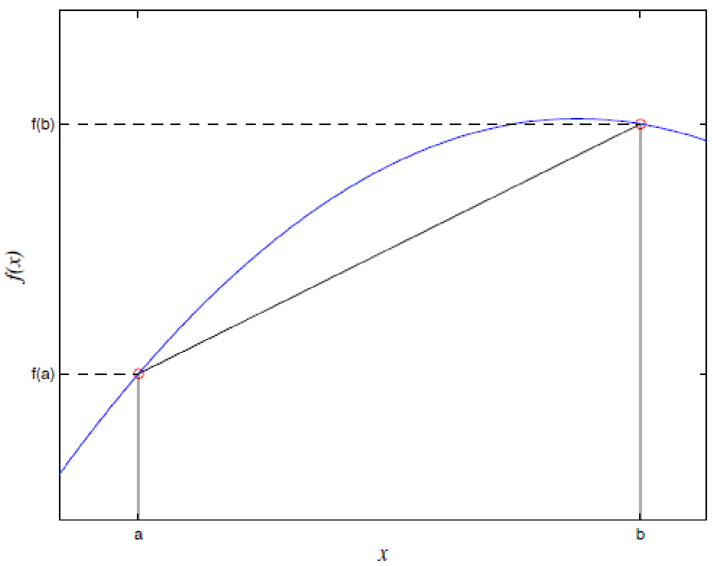

Figure 3.3 : Principle of trapezoidal rule.

The integral of this function can be found by a simple measurement of the area of the trapezoid with the long base $f(x_i)$, the short base $f(x_f)$; and the height $h = x_i - x_f$.

$$\int_{x_i}^{x_f} f(x)\,dx = \frac{h}{2}\left[f(x_i) + f(x_f)\right] \quad (1)$$

This approximation is too simple; we neglected a large area between the curve and the side of the trapezoid (Figure 3.3), so the calculated area is different from the exact one.

To reduce this error, we divide the domain into several equal domains.

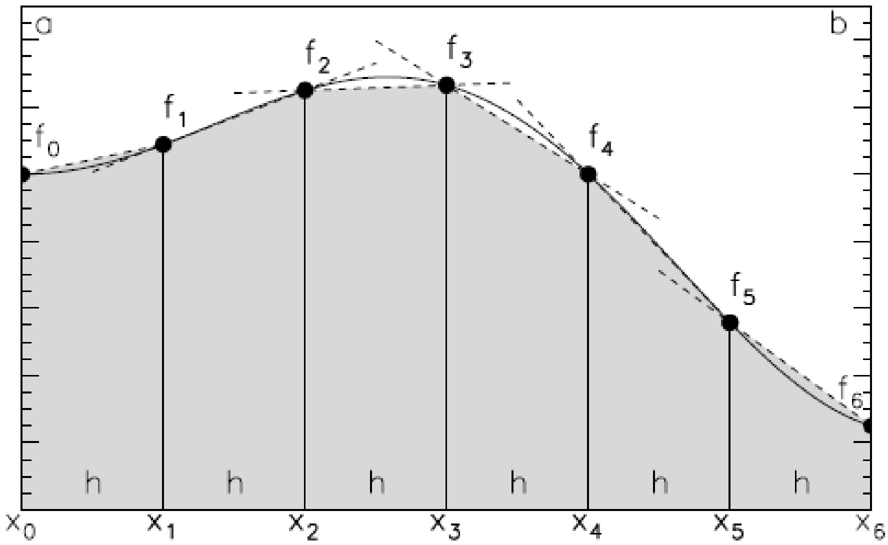

Figure 3.4 : Generalized Trapezoidal rule

Dividing the interval into n sub-intervals, the base of each trapezoid will be equal to $h = \frac{(x_f - x_i)}{n}$. So,

. The area of the first trapezoid is equal to $s_1 = \frac{h}{2}(f(x_i) + f(x_1))$.

. The area of the second trapezoid is equal to $s_2 = \frac{h}{2}(f(x_1) + f(x_2))$.

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. The area of (n-1) trapezoid is equal to $s_{n-1} = \frac{h}{2}(f(x_{n-2}) + f(x_{n-1}))$.

. The area of (n) trapezoid is equal to $s_n = \frac{h}{2}(f(x_{n-1}) + f(x_n))$.

Finally, the surface under the curve limited by the interval$[x_0, x_f]$ is the sum of all the surfaces of the trapezoids constituting this surface.

$$I_{trap} = \sum_{i=1}^{n} s_i$$

$$I_{trap} = \frac{h}{2}[f(x_i) + f(x_1) + f(x_1) + f(x_2) + \cdots\ f(x_{n-1}) + f(x_n)]$$

$$I_{trap} = \frac{h}{2}[f(x_1) + f(x_n) + 2\ \sum_2^{n-1} f(x_i)] \qquad (2)$$

Notes :

- The first formula (eq. 3.1) is often called the Simple Trapezoidal Method.
- The second formula (eq.3.2) is called the generalized trapezoidal method.

The error made on the value of the integral using this method is given by the expression,

$$E_{trap} = -\frac{(x_i - x_f)}{12} h^2\ f''(\delta),\ \ \delta \in [x_0, x_f]$$

$f''(\xi)$ represents the maximum value of the second derivative of the function on the interval $[x_i, x_f]$. We put:

$M_2 = \max_{\delta \in [x_0, x_f]} |f''(\delta)|,\ \ h = \frac{(x_f - x_i)}{n}$. Then,

$$\left|\boldsymbol{E_{trap}}\right| \leq \frac{\boldsymbol{(x_f - x_i)^3}}{\boldsymbol{12n^2}} \boldsymbol{M_2}$$

Example

Let's take a simple function$f(x) = \sqrt{x}$ and calculate its integral on the interval $[1, 3]$.

$I_{anly} = \frac{2}{3}x^{\left(\frac{3}{2}\right)}\Big]_1^3 = 2.7974.$

$$I_{trap}^{simple} = \frac{h}{2}[f(1) + f(3)], \qquad h = (3 - 1) = 2$$

$$I_{trap}^{simple} = \frac{2}{2}[1 + 1.7321] = 2.7321$$

If we divide the interval into 4 subintervals (we use generalized Simpson rule).

$$h = \frac{(3 - 1)}{4} = 0.5$$

$$I_{trap}^{gene} = \frac{0.5}{2}\left[f(1) + 2 \times \left(f\left(\frac{3}{2}\right) + f(2) + f\left(\frac{5}{2}\right)\right) + f(3)\right] = 2.7931$$

If we take,

$$n = 10, \quad h = \frac{(3 - 1)}{10} = 0.2, \qquad I_{trap}^{gene} = 2.7967$$

As n increases, the approximate value gets closer to the exact value.

Calculation of the error using the formula.

$$f(x) = \sqrt{x} \quad \rightarrow \; f'(x) = \frac{1}{2\sqrt{x}} \quad \rightarrow \; f''(x) = -\frac{1}{4}x^{3/2}$$

$$M_2 = \max_{\delta \in [x_0, x_f]} |f''(\xi)| \; \rightarrow \; \frac{1}{4}\left|\frac{1}{\left(\sqrt{1}\right)^3}\right| = \frac{1}{4}; (the\ maximun\ is\ at\ \delta = x = 1$$

$$n = 1, the\ error\ is$$

$$n = 4, the\ error\ is$$

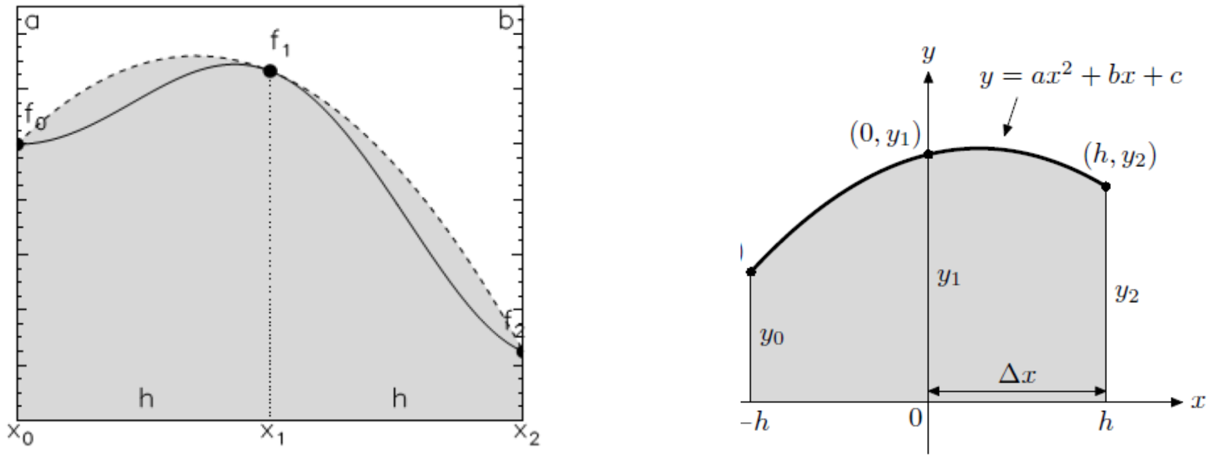
$$n = 10, the\ error\ is$$

3.3 Simpson rule:

Simpson's method of numerical integration consists of approximating the function f on the interval $[x_i, x_f]$ by a polynomial of second degree. The polynomial must coincide with the function at three points: the limits of the interval and the middle of the interval (fig.3.3a).

The polynomial that replaces the function on the interval I (fig.3.3b) is given by,

$$y = ax^2 + bx + c$$



(a) (b)

Figure 3.3 : Graphical representation of Simpson rule

Therefore, the integral of f is approximated by the integral of the polynomial $y = ax^2 + bx + c$.

$$I_{simp} = \int_{x_i}^{x_f} (ax^2 + bx + c)dx$$

Taking x_0 as the midpoint of the interval and h as the distance to the interval limit, the integral will be written as:

$$I_{simp} = \int_{x_0-h}^{x_0+h} (ax^2 + bx + c)dx$$

$$I_{simp} = \left[\frac{a}{3}x^3 + \frac{b}{2}x^2 + cx\right]_{x_0-h}^{x_0+h}$$

$$I_{simp} = \left(\frac{a}{3}(x_0+h)^3 + \frac{b}{2}(x_0+h)^2 + c(x_0-h)\right) - \left(\frac{a}{3}(x_0-h)^3 + \frac{b}{2}(x_0-h)^2 + c(x_0-h)\right)$$

We use these two expressions,

$$\begin{cases}(a+b)^3 = a^3 + b^3 + 3a^2b + 3ab^2 \\ (a-b)^3 = a^3 - b^3 - 3a^2b + 3ab^2\end{cases}$$

After rearrangement, we arrive to the formula

$$I_{simp} = \frac{h}{3}[ax_0^2 + 6bx_0 + 6c] \qquad 23$$

On the other hand, since the function coincides with the polynomial at (x_0-h), (x_0-h) and (x_0+h), we have:

$$f(x_0-h) = a(x_0-h)^2 + b(x_0-h) + c$$

$$f(x_0) = ax_0^2 + bx_0 + c$$

$$f(x_0+h) = a(x_0+h)^2 + b(x_0+h) + c$$

If we sum the last three equations in this way,

$$f(x_0-h) + 4f(x_0) + f(x_0+h),$$

We get the results,

$$f(x_0-h) + 4f(x_0) + f(x_0+h) = \frac{h}{3}[ax_0^2 + 6bx_0 + 6c] \qquad (24)$$

From formulas 23 and 24, we can write

$$I_{simp} = \frac{h}{3}[f(x_0-h) + 4f(x_0) + f(x_0+h)]$$

This formula is called Simpson's simple rule, since we replaced the function over the entire interval with a single polynomial. We can divide the interval into n subintervals and calculate the sum of these areas to better estimate the integral. This latter method is called the generalized Simpson method.

Note: As can be noted, Simpson's rule requires that the data set has an odd number of elements, resulting in an even number of intervals. This is why n must be an even number. $h = \frac{(x_i - x_f)}{n}$, so we have (n+1) points.

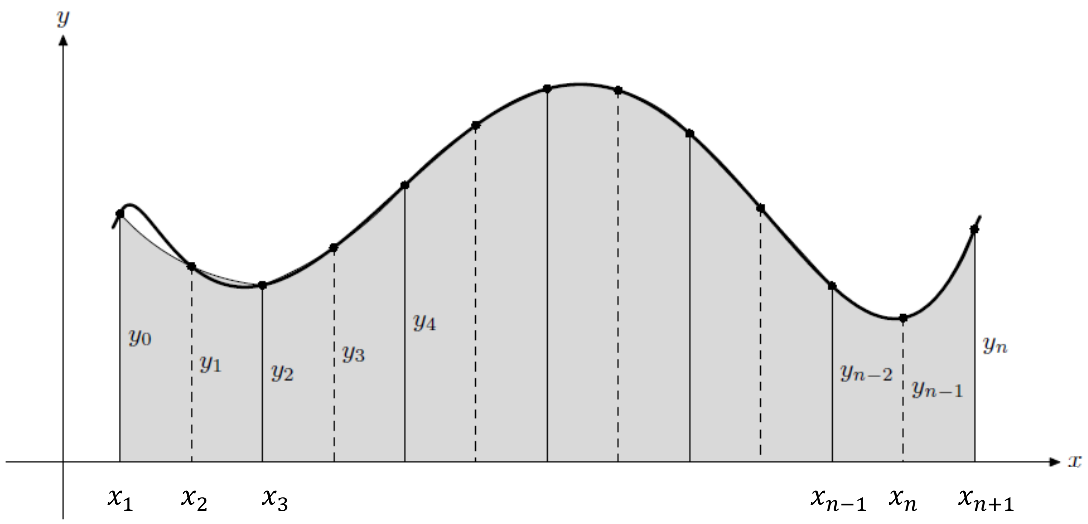


Figure 3.5: Graphical representation of generalized Simpson rule.

In the same way, we can estimate the integral with the sum of the integrals of each subdivision, $[\boldsymbol{x_1}, \boldsymbol{x_3}], [\boldsymbol{x_3}, \boldsymbol{x_5}], .. [\boldsymbol{x_{n-1}}, \boldsymbol{x_{n+1}}]$ by,

$$I_{simp} = \frac{h}{3}([f(x_1) + 4f(x_2) + f(x_3)] + [f(x_3) + 4f(x_4) + f(x_5)] + \cdots + [f(x_{n-1}) + 4f(x_n) + f(x_{n+1})])$$

By simplification, we find the generalized Simpson formula,

$$I_{simp} = \frac{h}{3}(f(x_1) + 4f(x_2) + 2f(x_3) + 4f(x_4) + 2f(x_5) + \cdots + 2f(x_{n-2}) + 4f(x_{n-1}) + f(x_{n+1})).$$

At last we can write,

$$I_{simp} = \frac{h}{3}\left[f(x_1) + 4\sum f(x_{even}) + 2\sum f(x_{odd}) + f(x_{n+1})\right]$$

Example

Find the integral of $\int_0^{\pi/2} \sin(x)dx$ represented by the table below.

X	0	$\pi/8$	$\pi/4$	$3\pi/8$	$\pi/2$
$f(x)$	0	0.382683	0.707107	0.923880	1

$$I_{simp} = \frac{h}{3}\left[f(0) + 2f(\frac{\pi}{4}) + 4\left(f\left(\frac{\pi}{8}\right) + f\left(\frac{3\pi}{8}\right)\right) + f(\frac{\pi}{2})\right]$$

$$= \frac{\pi}{8}\frac{1}{3}[0 + 4(0382683 + 0.92388) + 2(0,7071007) + 1] = 1.000135$$

The analytical integral is,

$$I = \int_0^{\pi/2} \sin x \, d\, x = 1$$

The difference between analytical and numerical results is $|s - I| = 0.000135.$

Error calculation of Simpson rule

The error made on the value of the integral using Simpson rule is given by the expression,

$$|\boldsymbol{E_{simp}}| = \frac{\boldsymbol{(x_i - x_f)h^4}}{\boldsymbol{180}} M_4$$

Where , $M_4 = \max_{\delta\in[a,b]} \left|f^{(4)}(\delta)\right|$ **,** then

$$\boldsymbol{|E_{Simp}| \leq \frac{(x_i - x_f)5}{180n^4} M_4}$$

Note :

In general, the Simpson rule gives a better approximation than the trapezoidal rule because the error made in the trapezoidal rule is proportional to h^2, while for Simpson it is proportional to h^4.