# COURSE 6

## 3. Numerical integration of functions

The need: for evaluating definite integrals of functions that has no explicit antiderivatives or whose antiderivatives are not easy to obtain.

Let $f : [a, b] \to \mathbb{R}$ be an integrable function, $x_k$, $k = 0, ..., m$, distinct nodes from $[a, b]$.

**Definition 1** *A formula of the form*

$$\int_a^b f(x)dx = \sum_{k=0}^{m} A_k f(x_k) + R(f),$$

*is* **a numerical integration formula** *or* **a quadrature formula**.

$A_k$ - **the coefficients**; $x_k$–**the nodes**; $R(f)$ - **the remainder (the error)**.

**Definition 2 Degree of exactness (degree of precision)** *of a quadrature formula is $r$ if and only if the error is zero for all the polynomials of degree $k = 0, 1, ..., r$, but is not zero for at least one polynomial of degree $r + 1$.*

From the linearity of $R$ we have that the degree of exactness is $r$ if and only if $R(e_i) = 0$, $i = 0, ..., r$ and $R(e_{r+1}) \neq 0$, where $e_i(x) = x^i$, $\forall i \in \mathbb{N}$.

## 3.1. Interpolatory quadrature formulas

**Definition 3** *A quadrature formula*

$$\int_a^b f(x)dx = \sum_{k=0}^{m} A_k f(x_k) + R(f),$$

*is* **an interpolatory quadrature formula** *if it is obtained by integrating each member of an interpolation formula regarding the function $f$ and the nodes $x_k$.*

**Remark 4** *An interpolatory quadrature formula has its degree of exactness at least the degree of the corresponding polynomial.*

Consider Lagrange interpolation formula regarding the nodes $x_k \in [a,b]$, $k = 0, ..., m$ :

$$f(x) = \sum_{k=0}^{m} \ell_k(x) f(x_k) + (R_m f)(x).$$

Integrating the two parts of this formula one obtains

$$\int_a^b f(x)dx = \sum_{k=0}^{m} A_k f(x_k) + R_m(f), \tag{1}$$

where

$$A_k = \int_a^b \ell_k(x)dx$$

and

$$R_m(f) = \int_a^b (R_m f)(x)dx. \tag{2}$$

If the nodes are equidistant, i.e., $x_k = a + kh$, $h = \frac{b-a}{m}$ then

$$A_k = (-1)^{m-k} \frac{h}{k!(m-k)!} \int_0^m \frac{t(t-1)...(t-m)}{(t-k)} dt, \;\; k = 0, ..., m. \tag{3}$$

The remainder from the Lagrange interpolation formula can be written as:

$$(R_m f)(x) = \frac{u(x)}{(m+1)!} f^{(m+1)}(\xi(x)),$$

where $u(x) = \prod_{k=0}^{m} (x - x_k)$, so the remainder of the quadrature formula may be written as

$$R_m(f) = \frac{1}{(m+1)!} \int_a^b u(x) f^{(m+1)}(\xi(x)) dx. \tag{4}$$

**Definition 5** *The quadrature formulas with equidistant nodes are called* **Newton-Cotes formulas.**

Consider the case $m = 1$ $(x_0 = a, x_1 = b, h = b - a)$.

Lagrange polynomial is

$$(L_1 f)(x) = \frac{x-b}{a-b} f(a) + \frac{x-a}{b-a} f(b)$$

and the remainder in interpolation formula is

$$(R_1 f)(x) = \frac{(x-a)(x-b)}{2} f''(\xi(x)).$$

Integrating the interpolation formula $f(x) = (L_1 f)(x) + (R_1 f)(x)$ one obtains

$$\int_a^b f(x)dx = \int_a^b \left[\frac{x-b}{a-b} f(a) + \frac{x-a}{b-a} f(b)\right] dx$$
$$+ \int_a^b \frac{(x-a)(x-b)}{2} f''(\xi(x)) dx.$$

As $(x-a)(x-b)$ does not change the sign, by *Mean Value Th.* (If f:[a, b]$\rightarrow$R is continuous and g is an integrable function that does not change sign on [a, b], then there exists c in (a, b) such that $\int_a^b f(x)g(x)dx = f(c) \int_a^b g(x)dx$), we have

$$\int_a^b f(x)dx = \left[\frac{(x-b)^2}{2(a-b)}f(a) + \frac{(x-a)^2}{2(b-a)}f(b)\right]\Bigg|_a^b$$
$$+ \frac{f''(\xi)}{2}\left[\frac{x^3}{3} - \frac{(a+b)x^2}{2} + abx\right]\Bigg|_a^b, \quad \xi \in (a,b).$$

We obtain **the trapezium's quadrature formula**

$$\int_a^b f(x)dx = \frac{b-a}{2}[f(a)+f(b)] - \frac{(b-a)^3}{12}f''(\xi). \tag{5}$$

This formula is called the trapezium's formula because the integral is approximated by the area of a trapezium.

**Remark 6** *The error from (5) involves $f''$, so the rule gives exact result when is applied to function whose second derivative is zero (polynomial of first degree or less). So its degree of exactness is 1.*

**Example 7** *Approximate the integral $\int_1^3 (2x+1)dx$ using the trapezium's formula.*

(*Remark.* The result is the exact value of the integral because $f(x) = 2x + 1$ is a linear function and the degree of exactness of the trapezium's formula is $1$.)

For $m = 2$ (($x_0 = a, x_1 = a + \frac{b-a}{2}, x_2 = b, h = \frac{b-a}{2}$) one obtains **the Simpson's quadrature formula**

$$\int_a^b f(x)dx = \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right] + R_2(f), \tag{6}$$

where

$$R_2(f) = -\frac{(b-a)^5}{2880} f^{(4)}(\xi),\ a \le \xi \le b. \tag{7}$$

**Remark 8** *The error from (6) involves $f^{(4)}$, so the rule gives exact result when is applied to any polynomial of third degree or less. So degree of exactness of Simpson's formula is 3.*

**Remark 9** *A Newton-Cotes quadrature formula has degree of exactness equal to* $\begin{cases} m, & \text{if } m \text{ is an odd number} \\ m+1, & \text{if } m \text{ is an even number.} \end{cases}$

**Remark 10** *The coefficients of the Newton-Cotes quadrature formulas have the symmetry property:*

$$A_i = A_{m-i}, i = 0, ..., m.$$

**Example 11** *Compare the trapezium's rule and Simpson's rule approximations for*

$$\int_0^2 x^2 dx.$$

**Sol.** *The exact value is* 2.667*; for trapezium rule the value is* 4*, for Simpson's rule the value is* 2.667*. (The approximation from Simpson's rule is exact because the error involves* $f^{(4)}(x) = 0$.*)*

**Example 12** *Approximate the integral using Simpson' s formula*

$$I = \int_0^4 e^x dx.$$

*(The real value is* $e^4 - 1 = 53.59$.*)*

**Sol.** We have $I \approx \frac{4}{6}\left[e^0 + 4e^2 + e^4\right] = 56.76.$

If we apply Simpson's formula twice we get

$$I \approx \int_0^2 e^x dx + \int_2^4 e^x dx \approx \frac{2}{6}\left[e^0 + 4e + e^2\right] + \frac{2}{6}\left[e^2 + 4e^3 + e^4\right] = 53.86$$

and if we apply four times we get

$$I \approx \sum_{i=0}^{3} \int_i^{i+1} e^x dx = 53.61,$$

so it follows the utility of using repeated formulas.

## 3.2. Repeated quadrature formulas.

In practice, the problem of approximating $I = \int_a^b f(x)dx$ can be set in the following way: approximate the integral $I$ with an absolute error not larger than a given bound $\varepsilon$.

By the trapezium's formula, for example, it follows that

$$|R_1(f)| = \frac{(b-a)^3}{12} |f"(\xi)| \geq \frac{(b-a)^3}{12} m_2 f$$

where $m_2 f = \min_{a \leq x \leq b} |f"(x)|$. Therefore, if

$$\varepsilon < \frac{(b-a)^3}{12} m_2 f$$

then the problem cannot be solved by the trapezium's formula.

A solution: use formula with higher degree of exactness (e.g., the Simpson formula, etc.). But as $m$ increases, the application of the formula becomes more difficult (computation, evaluation of the remainders (appear the derivatives of order $(m+1)$ or $(m+2)$ of $f$)).

An efficient way of constructing a practical quadrature formula: repeated application of a simple formula.

Let $x_k = a + kh,\ k = 0, ..., n$ with $h = \frac{b-a}{n}$, be the nodes of a uniform grid of $[a, b]$. By the additivity property of the integral we have

$$\int_a^b f(x)dx = \sum_{k=1}^{n} I_k, \text{ with } I_k = \int_{x_{k-1}}^{x_k} f(x)dx$$

Applying a quadrature formula to $I_k$, one obtains **the repeated quadrature formula.**

Applying to each integral $I_k$ the trapezium's formula, we get

$$\int_a^b f(x)dx = \sum_{k=1}^{n} \left\{ \frac{x_k - x_{k-1}}{2} \left[ f(x_{k-1}) + f(x_k) \right] - \frac{(x_k - x_{k-1})^3}{12} f''(\xi_k) \right\},$$

where $x_{k-1} \leq \xi_k \leq x_{k+1}$, or

$$\int_a^b f(x)dx = \frac{b-a}{2n}\left[f(a) + f(b) + 2\sum_{k=1}^{n-1} f(x_k)\right] + R_n(f), \tag{8}$$

with

$$R_n(f) = -\frac{(b-a)^3}{12n^3}\sum_{k=1}^{n} f''(\xi_k).$$

There exists $\xi \in (a, b)$ such that

$$\frac{1}{n}\sum_{k=1}^{n} f''(\xi_k) = f''(\xi).$$

So **the repeated trapezium's quadrature formula** is

$$\int_a^b f(x)dx = \frac{b-a}{2n}\left[f(a) + f(b) + 2\sum_{k=1}^{n-1} f(x_k)\right] + R_n(f), \tag{9}$$

with

$$R_n(f) = -\frac{(b-a)^3}{12n^2} f''(\xi),\ \ a < \xi < b \tag{10}$$

We have

$$|R_n(f)| \leq \frac{(b-a)^3}{12n^2} M_2 f,$$

where $M_2 f = \max\limits_{a \leq x \leq b} |f''(x)|$. By

$$|R_n(f)| \leq \frac{(b-a)^3}{12n^2} M_2 f, \tag{11}$$

it follows that the repeated trapezium quadrature formula allows the approx. of an integral with arbitrary small given error, if $n$ is taken sufficiently large. If we want that the absolute error to be smaller than $\varepsilon$, we determine the smallest solution $n$ of the inequation

$$\frac{(b-a)^3}{12n^2} M_2 f < \varepsilon, \ n \in \mathbb{N},$$

and using this value in (8), leads to desired approximation.

Similarly, there is obtained **the repeated Simpson's quadrature formula**

$$\int_a^b f(x)dx = \tfrac{b-a}{6n}\left[f(a)+f(b)+4\sum_{k=1}^{n} f\left(\tfrac{x_{k-1}+x_k}{2}\right)+2\sum_{k=1}^{n-1} f(x_k)\right]+R_n(f) \tag{12}$$

where

$$R_n(f) = -\frac{(b-a)^5}{2880n^4}f^{(4)}(\xi),\ \ a<\xi<b,$$

and

$$|R_n(f)| \le \frac{(b-a)^5}{2880n^4}M_4 f.$$

**Example 13** *Approximate the integral* $\int_1^3 (2x+1)dx$ *with repeated trapezium's formula for* $n=2$.

(*Remark.* The result is the exact value of the integral because $f(x)=2x+1$ is a linear function and the degree of exactness of the trapezium's formula is $1$.)

**Example 14** *Approximate* $\frac{\pi}{4}$ *with repeated trapezium's formula, considering precision* $\varepsilon = 10^{-2}$.

**Solution 15** *We have*

$$\frac{\pi}{4} = arctg(1) = \int_0^1 \frac{dx}{1+x^2},$$

*so* $f(x) = \frac{1}{1+x^2}$. *Using (11), we get*

$$|R_n(f)| \leq \frac{(1-0)^3}{12n^2} M_2 f.$$

*We have*

$$f'(x) = \frac{-2x}{(1+x^2)^2}$$

$$f''(x) = \frac{6x^2-2}{(1+x^2)^3}$$

*and*

$$M_2 f = \max_{x\in[0,1]} |f''(x)| = 2,$$

*so*

$$|R_n(f)| \leq \frac{1}{6n^2} < 10^{-2} \Rightarrow n^2 > \frac{10^2}{6} = 16.66 \Rightarrow n = 5.$$

*We have* $x_0 = 0, x_1 = \frac{1}{5}, x_2 = \frac{2}{5}, x_3 = \frac{3}{5}, x_4 = \frac{4}{5}, x_5 = 1$ $(h = \frac{1}{5})$. *The integral will be*

$$\int_a^b f(x)dx \approx \frac{1}{10}\left\{f(0) + f(1) + 2\left[f(\frac{1}{5}) + f(\frac{2}{5}) + f(\frac{3}{5}) + f(\frac{4}{5})\right]\right\} = 0.7837.$$

*(The real value is 0.7854.)*

**Example 16** *Approximate*

$$\ln 2 = \int_0^1 \frac{1}{1+x}dx,$$

*with precision* $\varepsilon = 10^{-3}$, *using the repeated Simpson's formula.*

**Solution 17** *We have* $f(x) = \frac{1}{1+x}$ *and* $f^{(4)}(x) = \frac{4!}{(1+x)^5}$. *It follows* $|f^{(4)}(\xi)| \leq 4! = 24,$ *for* $\xi \in [0,1]$.

$$|R_2(f)| \leq \frac{24}{2880n^4} = \frac{1}{120n^4} < 10^{-3} \Rightarrow n = 2.$$

*Therefore,* $x_k = kh,\ k = 0, ..., 2;\ h = \frac{1}{2}$, *so* $x_0 = 0,\ x_1 = \frac{1}{2};\ x_2 = 1$

$$\begin{aligned} \ln 2 &= \frac{1}{12}\left[f(0) + 4\left(f(\frac{1}{4}) + f(\frac{3}{4})\right) + 2f(\frac{1}{2}) + f(1)\right] \\ &= \frac{1}{12}\left[1 + 4\left(\frac{4}{5} + \frac{4}{7}\right) + \frac{4}{3} + \frac{1}{2}\right] \\ &\approx 0.693 \qquad (\textit{the real value is } 0.6931). \end{aligned}$$