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 degree of exactness at least 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:

$$(R_m f)(x)=\frac{u(x)}{(m+1)!}f^{(m+1)}(\xi(x)),\qquad \xi(x)\in[a,b]$$

where $u(x)=\prod_{k=0}^m (x-x_k)$, so the remainder of the quadrature formula (2) 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 formula (1) with equidistant nodes, i.e., with coefficients (3), is called* **a Newton-Cotes formula.**

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

Lagrange polynomial is

$$(L_1f)(x) = \frac{x-b}{a-b}f(a) + \frac{x-a}{b-a}f(b)$$

and the remainder in interpolation formula is

$$(R_1f)(x) = \frac{(x-a)(x-b)}{2}f''(\xi(x)).$$

Integrating the interpolation formula $f(x) = (L_1f)(x) + (R_1f)(x)$ one obtains

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

As $(x-a)(x-b)$ does not change the sign, by Mean Value Th. we have

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

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 degree one 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 degree three 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 ε.

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

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

where $m_2 f = \min\limits_{a \leq x \leq b} \left|f''(x)\right|$. 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

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

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

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

with

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

We have

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

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

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

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 ε, 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**

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

where

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

and

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

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.)