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 interpolation 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

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

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

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

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 that there exist $\xi \in (a,b)$ such that

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

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 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

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

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* $f^{(4)}(x) = 0$.*)*