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 $u(x) = \prod_{k=0}^{m} (x - x_k)$, 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.

Example 6 *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.)

Remark 7 *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.*

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

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

Example 8 *Approximate the integral* $\int_1^3 (2x+1)dx$ *using the Simpson's formula.*

Remark 9 *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 10 *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 11 *The coefficients of the Newton-Cotes quadrature formulas have the symmetry property:*

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

For $m = 3$, **Newton's formula**

$$\int_a^b f(x)dx = \frac{b-a}{8}\left[f(a) + 3f\left(\frac{2a+b}{3}\right) + 3f\left(\frac{a+2b}{3}\right) + f(b)\right] + R_3(f),$$

with

$$R_3(f) = -\frac{(b-a)^5}{648} f^{(4)}(\xi).$$

Example 12 *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* $f^{(4)}(x) = 0$*.)*