COURSE 7

3.1. Interpolatory quadrature formulas

Definition 1 *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 2 *An interpolatory quadrature formula has its degree of exactness at least the degree of the corresponding interpolation polynomial.*

Definition 3 *The quadrature formulas with equidistant nodes, $x_k = a + kh$, $h = \frac{b-a}{m}$, 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

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

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

$$\int_a^b f(x)dx = \frac{b-a}{2}[f(a) + f(b)] + R_1(f), \tag{1}$$

where the remainder (the error) is

$$R_1(f) = -\frac{(b-a)^3}{12} f''(\xi), \quad \xi \in (a, b).$$

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

Remark 4 *The error from (1) 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 5 *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**

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

where

$$R_2(f) = -\frac{(b-a)^5}{2880} f^{(4)}(\xi),\ a \le \xi \le b. \tag{3}$$

Example 6 *Approximate the integral* $\int_1^3 (2x+1)dx$ *using Simpson's formula.*

Remark 7 *The error from (2) 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 8 *A Newton-Cotes quadrature formula has degree of exactness equal to* $\begin{cases} m, & \textit{if } m \textit{ is an odd number} \\ m+1, & \textit{if } m \textit{ is an even number.} \end{cases}$

Remark 9 *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 10 *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* $f^{(4)}(x) = 0$.*)*

3.2. Repeated quadrature formulas

Example 11 *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.

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

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

where $m_2 f = \min\limits_{a \leq x \leq b} |f''(x)|$. 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 $x_{k-1} \leq \xi_k \leq x_k$, or

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

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

$$\int_a^b f(x)dx = \frac{b-a}{2n}\left[f(a) + f(b) + 2\sum_{k=1}^{n-1} f(x_k)\right] + R_n(f), \tag{5}$$

with

$$R_n(f) = -\frac{(b-a)^3}{12n^2} f''(\xi),\ \ a < \xi < b \tag{6}$$

We have

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

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

$$|R_n(f)| \le \frac{(b-a)^3}{12n^2} M_2 f, \tag{7}$$

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 (4), leads to desired approximation.

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

$$\int_a^b f(x)dx = \tfrac{b-a}{6n} \left[f(a) + f(b) + 4 \sum_{k=1}^{n} f\left(\tfrac{x_{k-1}+x_k}{2} \right) + 2 \sum_{k=1}^{n-1} f(x_k) \right] + R_n(f) \tag{8}$$

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

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

Sol. 1. *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.

2. We have

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

so $f(x) = \frac{1}{1+x^2}$. Using (7), 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 13 *Approximate*

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

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