

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 $f : [a, b] \rightarrow \mathbb{R}$ be an integrable function, x_k , $k = 0, \dots, m$, 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 $k = 0, 1, \dots, r$, 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 $R(e_i) = 0$, $i = 0, \dots, r$ 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 $x_k \in [a, b]$, $k = 0, \dots, m$:

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

Integrating the two parts of this formula one obtains

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

where

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

and

$$R_m(f) = \int_a^b (R_m f)(x) dx. \quad (2)$$

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

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

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

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

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

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

As $(x-a)(x-b)$ does not change the sign, by *Mean Value Th.* (If $f:[a, b] \rightarrow \mathbb{R}$ 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

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

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

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

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**

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

where

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

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:*

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

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 $I \approx \frac{4}{6} [e^0 + 4e^2 + e^4] = 56.76$.

If we apply Simpson's formula twice we get

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

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

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

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 $x_k = a + kh$, $k = 0, \dots, n$ 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

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

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

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

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

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

with

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

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

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

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

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

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

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

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

where

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

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*

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

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

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

(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, $x_k = kh$, $k = 0, \dots, 2$; $h = \frac{1}{2}$, so $x_0 = 0$, $x_1 = \frac{1}{2}$; $x_2 = 1$

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