COURSE 7

3.2. Repeated quadrature formulas

Example 1 *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

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

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

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

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

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

with

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

We have

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

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

$$|R_n(f)| \leq \frac{(b-a)^3}{12n^2} M_2 f, \tag{4}$$

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 (1), leads to desired approximation.

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

$$\int_a^b f(x)dx = \tfrac{b-a}{6n}\left[f(a)+f(b)+4\sum_{k=1}^{n} f\left(\tfrac{x_{k-1}+x_k}{2}\right)+2\sum_{k=1}^{n-1} f(x_k)\right]+R_n(f) \tag{5}$$

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 2 *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* $\varepsilon = 10^{-2}$. *(The real value is 0.7854.)*

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 (4), 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

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

3.3. The Romberg's iterative generation method of a repeated quadrature formula

The presence of derivatives in the remainder $\Rightarrow$ difficulties in applicability to practical problems and to computer programs. There are preferred, in this sense, the iterative quadratures.

Consider the iterative generation method of a repeated formula by *the Romberg's method.*

In the case of the trapezium formula we have

$$Q_{T_0}(f) = \frac{h}{2}\left[f(a) + f(b)\right],\ h = b - a,$$

$Q_{T_0}(f)$ being the first element of the sequence.

We divide the interval $[a, b]$ in two equal parts, of length $\frac{h}{2}$ and applying to each subinterval $[a, a + \frac{h}{2}]$ and $[a + \frac{h}{2}, b]$ the trapezium formula we get

$$Q_{T_1}(f) = \frac{h}{4}\left[f(a) + 2f\left(a + \frac{h}{2}\right) + f(b)\right]$$

or

$$Q_{T_1}(f) = \frac{1}{2} Q_{T_0}(f) + hf\left(a + \frac{h}{2}\right).$$

Dividing now each previous divisions $[a, \frac{a+b}{2}]$ and $[\frac{a+b}{2}, b]$ in two equal parts, we obtain a division of the initial interval in $4 = 2^2$ equal parts, each of length $\frac{h}{4}$. Applying the repeated trapezium formula, we get

$$\begin{aligned} Q_{T_2}(f) &= \frac{h}{8}\left[f(a) + 2\sum_{i=1}^{3} f\left(a + \frac{ih}{4}\right) + f(b)\right] \qquad (6) \\ &= \frac{1}{2} Q_{T_1}(f) + \frac{h}{2^2}\left[f\left(a + \frac{1}{2^2}h\right) + f\left(a + \frac{3}{2^2}h\right)\right]. \end{aligned}$$

Continuing in an analogous manner, we get

$$Q_{T_k}(f) = \frac{1}{2} Q_{T_{k-1}}(f) + \frac{h}{2^k}\sum_{j=1}^{2^{k-1}} f\left(a + \frac{2j-1}{2^k}h\right), \ k = 1, 2, ... \qquad (7)$$

We obtain the sequence

$$Q_{T_0}(f), \ Q_{T_1}(f), ..., Q_{T_k}(f), ... \qquad (8)$$

which converges to the value $I = \int_a^b f(x)dx$.

We approximate the error by $\left|Q_{T_n}(f) - Q_{T_{n-1}}(f)\right|$. If we want to approximate I with error less than ε, we compute successively the elements of (8) until the first index for which

$$\left|Q_{T_n}(f) - Q_{T_{n-1}}(f)\right| \leq \varepsilon,$$

$Q_{T_n}(f)$ being the required value.

Similarly, one may iteratively generate the repeated Simpson's formula. Denoting by $Q_{S_k}(f)$ the Simpson's formula repeated k times, we have

$$Q_{S_k}(f) = \frac{1}{3}\left[4Q_{T_{k+1}}(f) - Q_{T_k}(f)\right], \; k = 0, 1, ...$$

where

$$Q_{S_0}(f) = \frac{h}{6}\left[f(a) + 4f\left(a + \frac{h}{2}\right) + f(b)\right]$$

is the Simpson's quadrature formula.

Another **Romberg's algorithm**, based on Aitken scheme:

$$
\begin{array}{llll}
T_{00} & & & \\
T_{10} & T_{11} & & \\
\dots & & & \\
T_{i0} & T_{i1} & \dots & T_{ii}
\end{array}
\tag{9}
$$

where the first column is computed by repeated trapezium rule and the other rows are computed by

$$
T_{i,j} = \frac{4^{-j} T_{i-1,j-1} - T_{i,j-1}}{4^{-j} - 1}. \tag{10}
$$

The columns, rows and diagonal all converge to the value of the integral; for smooth functions, the diagonal converges fastest.

The Romberg scheme computed using formula (10) contains in its first column the values of the repeated trapezium rule and in its second column the values of the Simpson's rule with 2^i intervals.

If we want to approximate I with error less than ε, we compute successively the lines of (9) until

$$\left|T_{i,i} - T_{i-1,i-1}\right| \leq \varepsilon,$$

$T_{i,i}$ being the required value.

3.4. Adaptive quadrature methods

The repeated integration methods require equidistant nodes. There are problems where the function contains both regions with large variations and with small variations. It is needed a smaller step for the regions with large variations than for the regions with small variations in order that the error to be uniformly distributed.

Such methods, which adapt the size of the step in accordance with the need, are called **adaptive quadrature methods**.

We present the method based on the repeated Simpson's quadrature formula.

Suppose we want to approximate with precision ε the integral

$$I = \int_a^b f(x)\,dx.$$

First step: we apply the Simpson's formula with the step $h = \frac{b-a}{2}$ ($x_0 = a$, $x_1 = a + h$, $x_2 = b$):

$$\begin{gathered}\int_a^b f(x)\,dx = \tfrac{b-a}{6}\Big(f(a) + 4f(a+\tfrac{h}{2}) + f(b)\Big) - \tfrac{(b-a)^5}{2880} f^{(4)}(\xi) = \\ := S(a,b) - \tfrac{h^5}{90} f^{(4)}(\xi)\end{gathered} \tag{11}$$

Then, we apply the Simpson's formula with the step $\frac{(b-a)}{4} = \frac{h}{2}$:

$$\begin{gathered}\int_a^b f(x)\,dx = \tfrac{h}{6}[f(a) + 4f(a+\tfrac{h}{2}) + 2f(a+h) + 4f(a+\tfrac{3h}{2}) \\ + f(b)] - \tfrac{h^5}{2^4 \cdot 90} f^{(4)}(\theta)\end{gathered}$$

$$\int_a^b f(x)\,dx = S\left(a, \tfrac{a+b}{2}\right) + S\left(\tfrac{a+b}{2}, b\right) - \tfrac{1}{16}\tfrac{h^5}{90} f^{(4)}(\theta) \tag{12}$$

We estimate the error without determining $f^{(4)}(\xi)$. We suppose $f^{(4)}(\xi) \simeq f^{(4)}(\theta)$. We get

$$S(a,b) - \tfrac{h^5}{90} f^{(4)}(\xi) = S\left(a, \tfrac{a+b}{2}\right) + S\left(\tfrac{a+b}{2}, b\right) - \tfrac{1}{16}\tfrac{h^5}{90} f^{(4)}(\xi),$$

whence

$$S\left(a,b\right)-S\left(a,\frac{a+b}{2}\right)-S\left(\frac{a+b}{2},b\right)=\frac{15}{16}\frac{h^5}{90}f^{(4)}\left(\xi\right),$$

or

$$\frac{h^5}{90}f^{(4)}\left(\xi\right)=\frac{16}{15}\left(S\left(a,b\right)-S\left(a,\frac{a+b}{2}\right)-S\left(\frac{a+b}{2},b\right)\right)$$

Replacing in (12) we get

$$\left|\int_a^b f\left(x\right)dx-S\left(a,\frac{a+b}{2}\right)-S\left(\frac{a+b}{2},b\right)\right|=\frac{1}{16}\frac{h^5}{90}f^{(4)}\left(\theta\right)$$
$$=\frac{1}{15}\left|S\left(a,b\right)-S\left(a,\frac{a+b}{2}\right)-S\left(\frac{a+b}{2},b\right)\right|$$

So the remainder of the approximation of I by $S\left(a,\frac{a+b}{2}\right)+S\left(\frac{a+b}{2},b\right)$ is 15 times smaller than the expression $\left|S\left(a,b\right)-S\left(a,\frac{a+b}{2}\right)-S\left(\frac{a+b}{2},b\right)\right|$. Hence, if

$$\left|S\left(a,b\right)-S\left(a,\frac{a+b}{2}\right)-S\left(\frac{a+b}{2},b\right)\right|<15\varepsilon,\text{ then} \tag{13}$$

$$\left|I-S\left(a,\frac{a+b}{2}\right)-S\left(\frac{a+b}{2},b\right)\right|<\varepsilon.$$

When (13) does not hold, the procedure is applied individually on $[a,(a+b)/2]$ and $[(a+b)/2,b]$ in order to determine if the approx. of the integral on each two subintervals is performed with error $\varepsilon/2$. If yes, the sum of these two approx. offer an approx. of I with precision ε. If on a subinterval it is not obtained the error $\varepsilon/2$, then we divide that subinterval and we analyze if the approx. on the resulted two subintervals has precision $\varepsilon/4$, and so on. This procedure of halfing is continued until the corresponding error is attained on each subinterval.

Algorithm: (the idea: "divide and conquer")

```
function I=adquad(a,b,er)
    I1=Simpson(a,b)
    I2=Simpson(a,(a+b)/2)+Simpson((a+b)/2,b)
  if |I1-I2|<15*er
      I=I2
      return
  else
      I=adquad(a,(a+b)/2,er/2)+adquad((a+b)/2,b,er/2)
  end
```

Remark 3 *For example, for evaluating the integral* $\int_1^3 \frac{100}{x^2}\sin\frac{10}{x}dx$ *with* $\varepsilon = 10^{-4}$, *repeated Simpson formula requires* 177 *function evaluations, nearly twice as many as adaptive quadrature.*

3.5. General quadrature formulas

Using the interpolation formulas, there are obtained a large variety of quadrature formulas.

In the case of some concrete applications, the choosing of the quadrature formula is made according to the information about the function f.

A general quadrature formula is given by:

$$\int_a^b f(x)dx = \sum_{k=0}^{m} \sum_{j \in I_k} A_{kj} f^{(j)}(x_k) + R(f).$$

For example, consider the Hermite interpolation formula for $f : [a, b] \to \mathbb{R}$, the nodes $x_k \in [a, b]$, $k = 0, ..., m$ multiple of orders $r_0, ..., r_m \in \mathbb{N}$,

$$f = H_n f + R_n f, \tag{14}$$

with $\dot{n} = m + r_0 + ... + r_m$, and

$$(H_n f)(x) = \sum_{k=0}^{m} \sum_{j=0}^{r_k} h_{kj} f^{(j)}(x_k),$$

h_{jk} being the Hermite fundamental polynomials.

Formula (14) generates the quadrature formula with multiple nodes:

$$\int_a^b f(x)dx = \sum_{k=0}^{m} \sum_{j=0}^{r_k} A_{kj} f^{(j)}(x_k) + R_n(f),$$

with

$$A_{kj} = \int_a^b h_{kj}(x)dx.$$

Similarly, there are obtained quadrature formulas starting to Birkhoff interpolation formulas.

Example 4 *If we know only the values of $f'(a)$ and $f(b)$ which is the corresponding quadrature formula?*

Sol. We have $f(x) = (B_1 f)(x) + (R_1 f)(x)$ with

$$(B_1 f)(x) = b_{01}(x) f'(a) + b_{10}(x) f(b). \tag{15}$$

Formula (15) generates the quadrature formula

$$\int_a^b f(x)dx = \sum_{k=0}^{1} \sum_{j=I_k} A_{kj} f^{(j)}(x_k) + R_1(f),$$

with

$$A_{01} = \int_a^b b_{01}(x)dx = -\frac{(b-a)^2}{2}$$
$$A_{10} = \int_a^b b_{10}(x)dx = (b-a).$$