COURSE 7

3.3. The Romberg's iterative generation method

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

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

Continuing in an analogous manner, we get

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

We obtain the sequence

$$Q_{T_0}(f),\ Q_{T_1}(f), ..., Q_{T_k}(f), ... \tag{3}$$

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 (3) 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:

$$\begin{array}{llll} T_{00} & & & \\ T_{10} & T_{11} & & \\ \ldots & & & \\ T_{i0} & T_{i1} & \ldots & T_{ii} \end{array} \tag{4}$$

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

$$T_{i,j} = \frac{4^{-j} T_{i-1,j-1} - T_{i,j-1}}{4^{-j} - 1}. \tag{5}$$

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 (5) contains in its first column the values of the repeated trapezium rule and in its second column the values of the Simpson's rule.

If we want to approximate I with error less than ε, we compute successively the lines of (4) 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 for $x_0 = a$, $x_1 = a + \frac{h}{2}$, $x_2 = b$, with $h = b - a$.

$$\int_a^b f(x)\,dx = \frac{b-a}{6}\left(f(a) + 4f(a + \frac{h}{2}) + f(b)\right) - \frac{(b-a)^5}{2880} f^{(4)}(\xi) \tag{6}$$

Denoting $S(a,b) := \frac{b-a}{6}\left(f(a) + 4f(a + \frac{h}{2}) + f(b)\right)$ we have

$$\int_a^b f(x)\,dx = S(a,b) - \frac{h^5}{90} f^{(4)}(\xi) \tag{7}$$

It may be proved that the error of approximating I by $S\left(a, a + \frac{h}{2}\right) + S\left(a + \frac{h}{2}, b\right)$ is 15 times smaller than the expression

$\left|S(a,b) - S\left(a, a + \frac{h}{2}\right) - S\left(a + \frac{h}{2}, b\right)\right|$. Hence, if

$$\left|S(a,b) - S\left(a, a + \frac{h}{2}\right) - S\left(a + \frac{h}{2}, b\right)\right| < 15\varepsilon, \text{ then} \tag{8}$$

$$\left|\int_a^b f(x)\,dx - S\left(a, a+\frac{h}{2}\right) - S\left(a+\frac{h}{2}, b\right)\right| < \varepsilon.$$

When (8) 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 1 *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, if we know only the values of $f'(a)$ and $f(b)$ which is the corresponding quadrature formula?

Using the Birkhoff interpolation formula

$$f(x) = (x-b)f'(a) + f(b) + (R_1 f)(x)$$

we obtain the quadrature formula

$$\int_a^b f(x)dx = A_0 f'(a) + A_1 f(b) + R_1(f),$$

with

$$A_0 = A_{01} = \int_a^b (x-b)dx = -\frac{(a-b)^2}{2}$$
$$A_1 = A_{10} = \int_a^b dx = b-a.$$

3.6. Quadrature formulas of Gauss type

All the previous rules can be written in the form

$$\int_a^b f(x)dx = \sum_{k=1}^{m} A_k f(x_k) + R_m(f), \tag{9}$$

where the coefficients A_k, $k = 1, ..., m$, do not depend on the function f. We have picked the nodes x_k, $k = 1, ..., m$ equispaced and have then calculated the coefficients A_k, $k = 1, ..., m$. This guarantees that the rule is exact for polynomials of degree $\leq m$.

It is possible to make such a rule exact for polynomials of degree $\leq 2m - 1$, by choosing also the nodes appropriately. This is the basic idea of the gaussian rules.

Let $f : [a, b] \to \mathbb{R}$ be an integrable function and $w : [a, b] \to \mathbb{R}_+$ a weight function, integrable on $[a, b]$.

Definition 2 *A formula of the following form*

$$\int_a^b w(x)f(x)dx = \sum_{k=1}^{m} A_k f(x_k) + R_m(f) \tag{10}$$

is called **a quadrature formula of Gauss type** *or* **with maximum degree of exactness** *if the coefficients A_k and the nodes x_k, $k = 1, ..., m$ are determined such that the formula has the maximum degree of exactness.*

Remark 3 *The coefficients and the nodes are determined such that to minimize the error, to produce exact results for the largest class of polynomials.*

A_k and x_k, $k = 1, ..., m$ from (10) are $2m$ unknown parameters $\Rightarrow$ $2m$ equations obtained such that the formula (10) is exact for any polynomial degree at most $2m - 1$.

It is often possible to rewrite the integral $\int_a^b g(x)dx$ as $\int_a^b w(x)f(x)dx$, where $w(x)$ is a nonnegative integrable function, and $f(x) = \frac{g(x)}{w(x)}$ is smooth, or it is possible to consider the simple choice $w(x) = 1$.

For the general case, consider the elementary polynomials $e_k(x) = x^k$; $k = 0, ..., 2m-1$ and obtain the system s.t. $R_m(e_k) = 0$:

$$\begin{cases} \sum\limits_{k=1}^{m} A_k e_0(x_k) = \int_a^b w(x) e_0\,(x)\,dx \\ \sum\limits_{k=1}^{m} A_k e_1(x_k) = \int_a^b w(x) e_1\,(x)\,dx \\ ... \\ \sum\limits_{k=1}^{m} A_k e_{2m-1}(x_k) = \int_a^b w(x) e_{2m-1}\,(x)\,dx \end{cases}$$

$\Longleftrightarrow$

$$\begin{cases} A_1 + A_2 + ... + A_m = \mu_0 \\ A_1 x_1 + A_2 x_2 + ... + A_m x_m = \mu_1 \\ ... \\ A_1 x_1^{2m-1} + A_2 x_2^{2m-1} + ... + A_m x_m^{2m-1} = \mu_{2m-1} \end{cases} \tag{11}$$

with

$$\mu_k = \int_a^b w(x) x^k dx.$$

As, the system (11) is difficult to solve, there have been found other ways to find the unknown parameters.

If $w(x) = 1$ (this case was studied by Gauss), then the nodes are the roots of Legendre orthogonal polynomial

$$u(x) = \frac{m!}{(2m)!} [(x-a)^m (x-b)^m]^{(m)}$$

and for finding the coefficients we use the first m equations from the system (11).

For example, for $m = 2$, the interval $[-1, 1]$ and $w(x) = 1$, we get the system

$$\begin{cases} A_1 + A_2 = \int_{-1}^{1} dx = 2 \\ A_1 x_1 + A_2 x_2 = \int_{-1}^{1} x dx = 0 \\ A_1 x_1^2 + A_2 x_2^2 = \int_{-1}^{1} x^2 dx = \frac{2}{3} \\ A_1 x_1^3 + A_2 x_2^3 = \int_{-1}^{1} x^3 dx = 0 \end{cases} \tag{12}$$

with solution $A_1 = A_2 = 1$ and $x_1 = -\frac{\sqrt{3}}{3}, x_2 = \frac{\sqrt{3}}{3}$, which gives the fomula

$$\int_{-1}^{1} f(x) dx \simeq f(-\frac{\sqrt{3}}{3}) + f(\frac{\sqrt{3}}{3}).$$

This formula has degree of precision 3, i.e., it gives exact result for every polynomial of the 3−rd degree or less.

Remark 4 *The resulting rules look more complicated than the interpolatory rules. Both nodes and weights for gaussian rules are, in general, irrational numbers. But, on a computer, it usually makes no difference whether one evaluates a function at* $x = 3$ *or at* $x = 1/\sqrt{3}$. *Once the nodes and weights of such a rule are stored, these rules are as easily used as the trapezium rule or Simpson's rule. At the same time, these gaussian rules are usually much more accurate when compared with the last ones on the basis of number of function values used.*

Example 5 *Consider* $m = 1$ *and obtain the following Gauss type quadrature formula*

$$\int_a^b f(x)dx = A_1 f(x_1) + R_1(f).$$

The system (11) becomes

$$\begin{cases} A_1 = \int_a^b dx = b - a \\ A_1 x_1 = \int_a^b x dx = \frac{b^2 - a^2}{2}. \end{cases}$$

The unique solution of this system is $A_1 = b - a$, $x_1 = \frac{a+b}{2}$.

The same result is obtained considering x_1 *the root of the Legendre polynomial of the first degree,*

$$u(x) = \frac{1}{2}[(x-a)(x-b)]' = x - \frac{a+b}{2}.$$

The Gauss type quadrature formula with one node is

$$\int_a^b f(x)dx = (b-a)f\left(\frac{a+b}{2}\right) + R_1(f),$$

with

$$R_1(f) = \frac{(b-a)^3}{24} f''(\xi), \qquad \xi \in [a,b]$$

which is called **the rectangle quadrature rule** (also called **the mid-point rule).**

The repeated rectangle (midpoint) quadrature formula is

$$\int_a^b f(x)dx = \frac{b-a}{n} \sum_{i=1}^{n} f(x_i) + R_n(f),$$

$$R_n(f) = \frac{(b-a)^3}{24n^2} f''(\xi), \qquad \xi \in [a,b]$$

with $x_1 = a + \frac{b-a}{2n}$, $x_i = x_1 + (i-1)\frac{b-a}{n}$, $i = 2, ..., n.$

We have

$$|R_n(f)| \ \leq \frac{(b-a)^3}{24n^2} M_2 f, \quad \text{with } M_2 f = \max_{x \in [a,b]} |f''(x)|.$$

Remark 6 *Another* **rectangle rule** *is the following*:

$$\int_a^b f(x)dx = (b-a)f\,(a) + R(f),$$

with

$$R(f) = \frac{(b-a)^2}{2} f'(\xi), \qquad \xi \in [a,b].$$

Romberg's algorithm for the rectangle (midpoint) quadrature formula. Applying successively the rectangle formula on $[a, b]$, we get

$$Q_{D_0}(f) = (b-a)f(x_1), \quad x_1 = \frac{a+b}{2}$$

$$Q_{D_1}(f) = \frac{1}{3}Q_{D_0}(f) + \frac{b-a}{3}\left[f(x_2) + f\left(x_3\right)\right],$$

$$x_2 = a + \frac{b-a}{6},\ x_3 = b - \frac{b-a}{6}.$$

Continuing in an analogous manner, we obtain the sequence

$$Q_{D_0}(f),\ Q_{D_1}(f), ..., Q_{D_k}(f), ... \tag{13}$$

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

If we want to approximate the integral I with error less than ε, we compute successively the elements of (13) until the first index for which

$$\left|Q_{D_m}(f) - Q_{D_{m-1}}(f)\right| \leq \varepsilon,$$

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

The algorithm for generating the elements of the sequence (13) is:

I. Let $h := b - a$,$h_1 := \frac{h}{2}$,$x_1 : a + h_1$and $Q_{D_0}(f) := hf(x_1)$.

II. For $k := 1, 2$,... do

$h := \frac{h}{3}$,$h_1 := \frac{h_1}{3}$,$h_2 := 4h_1$,$h_3 := 2h_1$, $m := 3^{k-1}$,$x_1 := a + h_1$;

for $i = 1, ..., m - 1$,do $x_{2i} := x_{2i-1} + h_{2,}x_{2i+1} := x_{2i} + h_3$;

$x_{2m} := x_{2m-1} + h_2$ and

$$Q_{D_k}(f) = \frac{1}{3}Q_{D_{k-1}}(f) + h\sum_{i=1}^{2m} f(x_i),$$

(for $k = 1(m = 1)$the generation of x_{2i},$x_{2i+1}$is missing).

Example 7 *Approximate* $\ln 2$*, with* $\varepsilon = 10^{-2}$*, using the repeated rectangle (midpoint) method.*

Solution. We have

$$\int_a^b f(x)dx = \frac{b-a}{n}\sum_{i=1}^{n} f(x_i) + R_n(f),$$

$$R_n(f) = \frac{(b-a)^3}{24n^2}f''(\xi), \qquad \xi \in [a,b].$$

$$\ln 2 = \int_1^2 \frac{dx}{x},$$

so $f(x) = \frac{1}{x}$ and we get

$$\ln 2 = \frac{b-a}{n}\left[f(a+\frac{b-a}{2n}) + \sum_{i=2}^{n} f(a+\frac{b-a}{2n}+(i-1)\frac{b-a}{n})\right] + \frac{(b-a)^3}{24n^2}f''(\xi)$$

We have $f(x) = \frac{1}{x}$, $f'(x) = -\frac{1}{x^2}$, $f''(x) = \frac{2}{x^3}$, and $|f''(\xi)| \leq 2$, for $\xi \in [1,2]$ so it follows

$$|R_n(f)| \leq \frac{1}{24n^2}2 < 10^{-2} \Rightarrow 12n^2 > 100 \Rightarrow n = 3.$$

Therefore,

$$\ln 2 \approx \frac{1}{3}\left(\frac{1}{1+\frac{1}{6}}+\frac{1}{1+\frac{1}{6}+\frac{1}{3}}+\frac{1}{1+\frac{1}{6}+\frac{2}{3}}\right)=\frac{1}{3}\left(\frac{6}{7}+\frac{6}{9}+\frac{6}{11}\right)=0.6897$$

(real value is 0.693...)