3. Numerical integration of functions (continuation)

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)**.

Example 2 *Approximate*

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

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

Solution 3 *We have* $f(x)=\frac{1}{1+x}$ *and* $f^{(4)}(x)=\frac{4!}{(1+x)^5}$. *It follows* $|f^{(4)}(\xi)|\le 4!=24$, *for* $\xi\in[0,1]$.

$$|R_2(f)|\le\frac{24}{2880n^4}=\frac{1}{120n^4}<10^{-3}\Rightarrow n=2.$$

Therefore, $x_k=kh$, $k=0,...,2$; $h=\frac{1}{2}$, *so* $x_0=0$, $x_1=\frac{1}{2}$; $x_2=1$

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

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

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

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

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

$Q_{T_n}(f)$ 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.

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 $h = b - a$.

$$\begin{aligned}\textstyle\int_a^b f(x)\, dx = \frac{b-a}{6}\left(f(a) + 4f(a + \frac{h}{2}) + f(b)\right) - \frac{(b-a)^5}{2880} f^{(4)}(\xi) = \\ := S(a,b) - \frac{h^5}{90} f^{(4)}(\xi)\end{aligned} \tag{4}$$

It may be proved that the remainder of the approximation of I by $S\left(a, a + \frac{h}{2}\right) + S\left(a + \frac{h}{2}, b\right)$, $h = b - a$ 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

$$\left|S(a,b) - S\left(a, a + \tfrac{h}{2}\right) - S\left(a + \tfrac{h}{2}, b\right)\right| < 15\varepsilon, \text{ then} \tag{5}$$

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

When (5) 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 4 *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 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. General quadrature formula:

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

For example, if we know only the values of $f'(a)$ and $f(b)$, using the Birkhoff interpolation formula

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

we obtain the quadrature formula

$$\begin{aligned}\int_a^b f(x)dx &= A_0 f'(a) + A_1 f(b)\\ &= (b-a)\left[\frac{a-b}{2}f'(a) + f(b)\right] + R_1(f),\end{aligned}$$

with

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

3.6. Quadrature formulas of Gauss type

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 5 *A quadrature formula of the following form*

$$\int_a^b w(x)f(x)dx = \sum_{k=1}^{m} A_k f(x_k) + R_m(f) \qquad (6)$$

is called 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 6 *The coefficients and the nodes are determined such that to minimize the error, to produce exact result for the largest class of polynomials.*

A_k and x_k, $k=1,...,m$ from (6) are $2m$ unknown parameters $\Rightarrow$ $2m$ equations obtained such that the formula (6) is exact for any polynomial degree at most $2m-1$.

To illustrate we consider an example for $m = 2$. The integration formula

$$\int_{-1}^{1} f(x)dx \simeq A_1 f(x_1) + A_2 f(x_2)$$

gives exact result whenever $f(x)$ is a polynomial of degree $2 \cdot 2 - 1 = 3$ or less, i.e., $f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3$. Because

$$\int (a_0 + a_1 x + a_2 x^2 + a_3 x^3) dx = a_0 \int dx + a_1 \int x dx + a_2 \int x^2 dx + a_3 \int x^3 dx,$$

this is equivalent to showing that the formula is exact when $f(x)$ is $1, x, x^2$ and x^3. We get the system

$$\begin{cases} A_1 + A_2 = \int_{-1}^{1} dx = 2 \\ A_1 x_1 + A_2 x_2 = \int_{-1}^{1} x dx = 0 \\ A_1 x_1^2 + A_2 x_2^2 = \int_{-1}^{1} x^2 dx = \frac{2}{3} \\ A_1 x_1^3 + A_2 x_2^3 = \int_{-1}^{1} x^3 dx = 0 \end{cases} \quad (7)$$

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 degree 3 or less.

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

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

$\Longleftrightarrow$

$$\begin{cases} A_1 + A_2 + ... + A_m = \mu_0 \\ A_1 x_1 + A_2 x_2 + ... + A_m x_m = \mu_1 \\ \ldots \\ A_1 x_1^{2m-1} + A_2 x_2^{2m-1} + ... + A_m x_m^{2m-1} = \mu_{2m-1} \end{cases} \quad (8)$$

with

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

As, the system (8) 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 (8).

Example 7 *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 (8) 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 first degree,

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

The quadrature formula of Gauss type with one node is

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

which is also called **the rectangle quadrature formula.**

Example 8 *For $m = 2$, the quadrature formula is*

$$\int_a^b f(x)dx = A_1 f(x_1) + A_2 f(x_2) + R_2(f).$$

The corresponding Legendre polynomial is

$$u(x) = \frac{2}{4!}\left[(x-a)^2(x-b)^2\right]'' = x^2 - (a+b)x + \frac{1}{6}(a^2+b^2+4ab),$$

with the roots

$$x_1 = \frac{a+b}{2} - \frac{(b-a)\sqrt{3}}{6}, \quad x_2 = \frac{a+b}{2} + \frac{(b-a)\sqrt{3}}{6}.$$

For finding A_1 and A_2 we use the first two equations:

$$\begin{cases} A_1 + A_2 = b-a \\ A_1x_1 + A_2x_2 = (b^2-a^2)/2. \end{cases}$$

We get

$$A_1 = A_2 = (b-a)/2,$$

so the quadrature formula of Gauss type with two nodes is

$$\int_a^b f(x)dx = \frac{b-a}{2}\left[f\left(\frac{a+b}{2} - \frac{b-a}{6}\sqrt{3}\right) + f\left(\frac{a+b}{2} + \frac{b-a}{6}\sqrt{3}\right)\right] + R_2(f).$$

The repeated rectangle 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

$$|R_n(f)| \le \frac{(b-a)^3}{24n^2}M_2f, \quad \text{with } M_2f = \max_{x\in[a,b]}|f''(x)|.$$

Example 9 *Approximate* $\ln 2$*, with* $\varepsilon = 10^{-2}$*, using the repeated rectangle 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

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

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

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

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...)

Romberg's algorithm for rectangle quadrature formula. Apply successively the rectangle formula on $[a,b]$, then on subintervals obtained by dividing in 3 equal parts, in 3^2 equal parts, and so on. We get

$$Q_{D_0}(f) = (b-a)f(x_1), \quad x_1 = \frac{a+b}{2} \tag{9}$$

$$Q_{D_1}(f) = \frac{1}{3}Q_{D_0}(f) + \frac{b-a}{3}\left[f(x_2) + f(x_3)\right], \quad x_2 = a + \frac{b-a}{6}, \; x_3 = b - \frac{b}{}$$

Continuing in an analogous manner, we obtain the sequence

$$Q_{D_0}(f),\; Q_{D_1}(f), ..., Q_{D_k}(f), ... \tag{10}$$

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 (10) 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.