Chapter 4
Numerical Integration

Physical simulations often involve the calculation of definite integrals over complicated functions, for instance the Coulomb interaction between two electrons. Integration is also the elementary step in solving equations of motion.

An integral over a finite interval $[a, b]$ *can always be transformed into an integral over* $[0, 1]$ or $[-1, 1]$

$$\int_a^b f(x)dx = \int_0^1 f(a + (b - a)t)\,(b - a)dt$$
$$= \int_{-1}^1 f\left(\frac{a+b}{2} + \frac{b-a}{2}t\right)\frac{b-a}{2}dt. \tag{4.1}$$

An Integral over an infinite interval may have to be transformed into an integral over a finite interval by substitution of the integration variable, for example

$$\int_0^\infty f(x)dx = \int_0^1 f\left(\frac{t}{1-t}\right)\frac{dt}{(1-t)^2} \tag{4.2}$$
$$\int_{-\infty}^\infty f(x)dx = \int_{-1}^1 f\left(\frac{t}{1-t^2}\right)\frac{t^2+1}{(t^2-1)^2}dt. \tag{4.3}$$

In general a definite integral can be approximated numerically as the weighted average over a finite number of function values

$$\int_a^b f(x)dx \approx \sum_{x_i} w_i f(x_i). \tag{4.4}$$

Specific sets of quadrature points x_i *and quadrature weights* w_i *are known as "integral rules". Newton–Cotes rules like the trapezoidal rule, the midpoint rule or Simpson's rule, use equidistant points* x_i *and are easy to apply. Accuracy can be improved by dividing the integration range into sub-intervals and applying*

P.O.J. Scherer, *Computational Physics*, Graduate Texts in Physics,
DOI 10.1007/978-3-319-61088-7_4

composite Newton–Cotes rules. Extrapolation methods reduce the error almost to machine precision but need many function evaluations. Equidistant sample points are convenient but not the best choice. Clenshaw–Curtis expressions use non uniform sample points and a rapidly converging Chebyshev expansion. Gaussian integration fully optimizes the sample points with the help of orthogonal polynomials.

4.1 Equidistant Sample Points

For equidistant points

$$x_i = a + ih \quad i = 0 \ldots N \quad h = \frac{b-a}{N} \tag{4.5}$$

the interpolating polynomial of order N with $p(x_i) = f(x_i)$ is given by the Lagrange method

$$p(x) = \sum_{i=0}^{N} f_i \prod_{k=0,k\neq i}^{N} \frac{x - x_k}{x_i - x_k}. \tag{4.6}$$

Integration of the polynomial gives

$$\int_a^b p(x)dx = \sum_{i=0}^{N} f_i \int_a^b \prod_{k=0,k\neq i}^{N} \frac{x - x_k}{x_i - x_k} dx. \tag{4.7}$$

After substituting

$$\begin{aligned} x &= a + hs \\ x - x_k &= h(s-k) \\ x_i - x_k &= (i-k)h \end{aligned} \tag{4.8}$$

we have

$$\int_a^b \prod_{k=0,k\neq i}^{N} \frac{x - x_k}{x_i - x_k} dx = \int_0^N \prod_{k=0,k\neq i}^{N} \frac{s-k}{i-k} h ds = h\alpha_i \tag{4.9}$$

and hence

$$\int_a^b p(x)dx = (b-a) \sum_{i=0}^{N} f_i \alpha_i. \tag{4.10}$$

The weight factors are given by

$$w_i = (b - a)\alpha_i = Nh\alpha_i. \tag{4.11}$$

4.1.1 Closed Newton–Cotes Formulae

For $N = 1$ the polynomial is

$$p(x) = f_0 \frac{x - x_1}{x_0 - x_1} + f_1 \frac{x - x_0}{x_1 - x_0} \tag{4.12}$$

and the integral is

$$\begin{aligned}
&\int_a^b p(x)dx = f_0 \int_0^1 \frac{s-1}{0-1} h ds + f_1 \int_0^1 \frac{s-0}{1-0} h ds \\
&= -f_0 h \left(\frac{(1-1)^2}{2} - \frac{(0-1)^2}{2} \right) + f_1 h \left(\frac{1^2}{2} - \frac{0^2}{2} \right) \\
&= h \frac{f_0 + f_1}{2}
\end{aligned} \tag{4.13}$$

which is known as the trapezoidal rule (Fig. 4.1). $N = 2$ gives Simpson's rule

$$2h \, \frac{f_0 + 4f_1 + f_2}{6}. \tag{4.14}$$

Larger N give further integration rules

$$\begin{aligned}
&3h \, \frac{f_0 + 3f_1 + 3f_2 + f_3}{8} && 3/8 - \text{rule} \\
&4h \, \frac{7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4}{90} && \text{Milne} - \text{rule} \\
&5h \, \frac{19f_0 + 75f_1 + 50f_2 + 50f_3 + 75f_4 + 19f_5}{288} && \\
&6h \, \frac{41f_0 + 216f_1 + 27f_2 + 272f_3 + 27f_4 + 216f_5 + 41f_6}{840} && \text{Weddle} - \text{rule.}
\end{aligned} \tag{4.15}$$

For even larger N negative weight factors appear and the formulas are not numerically stable.

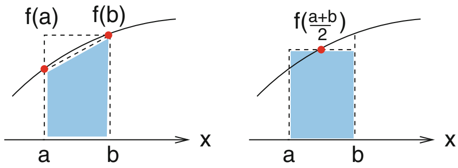

Fig. 4.1 (Trapezoidal rule and midpoint rule) The trapezoidal rule (***Left***) approximates the integral by the average of the function values at the boundaries. The midpoint rule (***Right***) evaluates the function in the center of the interval and has the same error order

4.1.2 Open Newton–Cotes Formulae

Alternatively, the integral can be computed from only interior points

$$x_i = a + ih \quad i = 1, 2, \ldots N \quad h = \frac{b-a}{N+1}. \tag{4.16}$$

The simplest case is the midpoint rule (Fig. 4.1)

$$\int_a^b f(x)dx \approx 2hf_1 = (b-a)f\left(\frac{a+b}{2}\right). \tag{4.17}$$

The next two are

$$\frac{3h}{2}\left(f_1 + f_2\right) \tag{4.18}$$

$$\frac{4h}{3}\left(2f_1 - f_2 + 2f_3\right). \tag{4.19}$$

4.1.3 Composite Newton–Cotes Rules

Newton–Cotes formulas are only accurate, if the step width is small. Usually the integration range is divided into small sub-intervals

$$[x_i, x_{i+1}] \quad x_i = a + ih \quad i = 0 \ldots N \tag{4.20}$$

for which a simple quadrature formula can be used. Application of the trapezoidal rule for each interval

$$I_i = \frac{h}{2}\left(f(x_i) + f(x_{i+1})\right) \tag{4.21}$$

gives the composite trapezoidal rule

$$T = h\left(\frac{f(a)}{2} + f(a+h) + \cdots f(b-h) + \frac{f(b)}{2}\right) \tag{4.22}$$

with error order $O(h^2)$. Repeated application of Simpson's rule for $[a, a+2h]$, $[a+2h, a+4h]\ldots$ gives the composite Simpson's rule

$$S = \frac{h}{3}\Big(f(a) + 4f(a+h) + 2f(a+2h) + 4f(a+3h) + \cdots + 2f(b-2h) + 4f(b-h) + f(b)\Big) \tag{4.23}$$

with error order $O(h^4)$.[1]

Repeated application of the midpoint rule gives the composite midpoint rule

$$M = 2h\left(f(a+h) + f(a+3h) + \cdots f(b-h)\right) \tag{4.24}$$

with error order $O(h^2)$.

4.1.4 Extrapolation Method (Romberg Integration)

For the trapezoidal rule the Euler–McLaurin expansion exists which for a $2m$ times differentiable function has the form

$$\int_{x_0}^{x_N} f(x)dx - T = \alpha_2 h^2 + \alpha_4 h^4 + \cdots \alpha_{2m-2} h^{2m-2} + O(h^{2m}). \tag{4.25}$$

Therefore extrapolation methods are applicable. From the composite trapezoidal rule for h and $h/2$ an approximation of error order $O(h^4)$ results:

[1] The number of sample points must be even.

$$\int_{x_0}^{x_N} f(x)dx - T(h) = \alpha_2 h^2 + \alpha_4 h^4 + \cdots \tag{4.26}$$

$$\int_{x_0}^{x_N} f(x)dx - T(h/2) = \alpha_2 \frac{h^2}{4} + \alpha_4 \frac{h^4}{16} + \cdots \tag{4.27}$$

$$\int_{x_0}^{x_N} f(x)dx - \frac{4T(h/2) - T(h)}{3} = -\alpha_4 \frac{h^4}{4} + \cdots \tag{4.28}$$

More generally, for the series of step widths

$$h_k = \frac{h_0}{2^k} \tag{4.29}$$

the Neville method gives the recursion for the interpolating polynomial

$$P_{i\cdots k}(h^2) = \frac{(h^2 - \frac{h_0^2}{2^{2i}}) P_{i+1\cdots k}(h^2) - (h^2 - \frac{h_0^2}{2^{2k}}) P_{i\cdots k-1}(h^2)}{\frac{h_0^2}{2^{2k}} - \frac{h_0^2}{2^{2i}}} \tag{4.30}$$

which for $h = 0$ becomes the higher order approximation to the integral (Fig. 4.2)

$$P_{i\cdots k} = \frac{2^{-2k} P_{i\cdots k-1} - 2^{-2i} P_{i+1\cdots k}}{2^{-2k} - 2^{-2i}} = \frac{P_{i\cdots k-1} - 2^{2k-2i} P_{i+1\cdots k}}{1 - 2^{2k-2i}}$$
$$= P_{i+1\cdots k} + \frac{P_{i\cdots k-1} - P_{i+1\cdots k}}{1 - 2^{2k-2i}}. \tag{4.31}$$

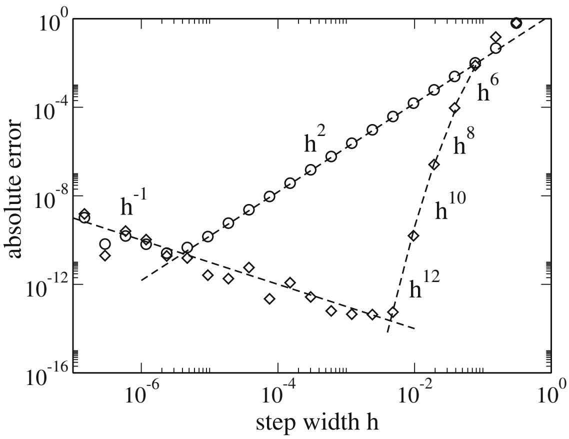

Fig. 4.2 (Romberg integration) The integral $\int_0^{\pi^2} \sin(x^2)dx$ is calculated numerically. *Circles* show the absolute error of the composite trapezoidal rule (4.22) for the step size sequence $h_{i+1} = h_i/2$. *Diamonds* show the absolute error of the extrapolated value (4.31). The error order of the trapezoidal rule is $O(h^2)$ whereas the error order of the Romberg method increases by factors of h^2. For very small step sizes the rounding errors dominate which increase as h^{-1}

The polynomial values can again be arranged in matrix form

$$\begin{array}{lll} P_0 & P_{01} & P_{012} \cdots \\ P_1 & P_{12} & \\ P_2 & & \\ \vdots & & \end{array} \tag{4.32}$$

with

$$T_{i,j} = P_{i \cdots i+j} \tag{4.33}$$

and the recursion formula

$$T_{i,0} = P_i = T_s\left(\frac{h_0}{2^i}\right) \tag{4.34}$$

$$T_{i,j} = T_{i+1,j-1} + \frac{T_{i,j-1} - T_{i+1,j-1}}{1 - 2^{2j}}. \tag{4.35}$$

4.2 Optimized Sample Points

The Newton–Cotes method integrates polynomials of order up to $N - 1$ exactly, using N equidistant sample points. Unfortunately the polynomial approximation converges slowly, at least for not so well behaved integrands. The accuracy of the integration can be improved by optimizing the sample point positions. Gaussian quadrature determines the N positions and N weights such, that a polynomial of order $2N - 1$ is integrated exactly. The Clenshaw–Curtis and the related Fejer methods use the roots or the extrema of the Chebyshev polynomials as nodes and determine the weights to integrate polynomials of order N. However, since the approximation by Chebyshev polynomials usually converges very fast, the accuracy is in many cases comparable to the Gaussian method [17, 18]. In the following we restrict the integration interval to $[-1, 1]$. The general case $[a, b]$ is then given by a simple change of variables.

4.2.1 Clenshaw–Curtis Expressions

Clenshaw and Curtis [19] make the variable substitution

$$x = \cos\theta \quad dx = -\sin\theta \, d\theta \tag{4.36}$$

for the integral

$$\int_{-1}^{1} f(x)dx = \int_{0}^{\pi} f(\cos t)\ \sin t\, dt \tag{4.37}$$

and approximate the function by the trigonometric polynomial (7.19 with $N = 2M, T = 2\pi$)

$$f(\cos t) = \frac{1}{2M}c_0 + \frac{1}{M}\sum_{j=1}^{M-1} c_j \cos(j\, t) + \frac{1}{2M}c_M \cos(Mt) \tag{4.38}$$

which interpolates (Sect. 7.2.1) $f(\cos t)$ at the sample points

$$t_n = n\Delta t = n\frac{\pi}{M} \quad \text{with} n = 0, 1, \ldots M \tag{4.39}$$

$$x_n = \cos t_n = \cos\left(n\frac{\pi}{M}\right) \tag{4.40}$$

and where the Fourier coefficients are given by (7.17)

$$c_j = f_0 + 2\sum_{n=1}^{M-1} f(\cos(t_n))\cos(\frac{\pi}{M} jn) + f_M \cos(j\pi). \tag{4.41}$$

The function $\cos(j\ t)$ is related to the Chebyshev polynomials of the first kind which for $-1 \le x \le 1$ are given by the trigonometric definition

$$T_j(x) = \cos(j\ \arccos(x)) \tag{4.42}$$

and can be calculated recursively

$$T_0(x) = 1 \tag{4.43}$$

$$T_1(x) = x \tag{4.44}$$

$$T_{j+1}(x) = 2x\, T_j(x) - T_{j-1}(x). \tag{4.45}$$

Substituting $x = \cos t$ we find

$$T_j(\cos t) = \cos(j\ t). \tag{4.46}$$

Hence the Fourier series (4.38) corresponds to a Chebyshev approximation

$$f(x) = \sum_{j=0}^{M} a_j T_j(x) = \frac{c_0}{2M} T_0(x) + \sum_{j=1}^{M-1} \frac{c_j}{M} T_j(x) + \frac{c_M}{2M} T_M(x) \tag{4.47}$$

and can be used to approximate the integral

$$\int_{-1}^{1} f(x)dx \approx \int_0^{\pi} \left\{ \frac{1}{2M} c_0 + \frac{1}{M} \sum_{j=1}^{M-1} c_j \cos(j\,t) + \frac{1}{2M} c_M \cos(Mt) \right\} \sin\theta \, d\theta \tag{4.48}$$

$$= \frac{1}{M} c_0 + \frac{1}{M} \sum_{j=1}^{M-1} c_j \frac{\cos(j\pi) + 1}{1 - j^2} + \frac{1}{2M} c_M \frac{\cos(M\pi) + 1}{1 - M^2} \tag{4.49}$$

where, in fact, only the even j contribute.

Example Clenshaw Curtis quadrature for $M = 5$

The function has to be evaluated at the sample points $x_k = \cos(\frac{\pi}{5} k) = (1, 0.80902, 0.30902, -0.30902, -0.80902, -1)$. The Fourier coefficients are given by

$$\begin{pmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \end{pmatrix} = \begin{pmatrix} 1 & 2 & 2 & 2 & 2 & 1 \\ 1 & 1.618 & 0.618 & -0.618 & -1.618 & -1 \\ 1 & 0.618 & -1.618 & -1.618 & 0.618 & 1 \\ 1 & -0.618 & -1.618 & 1.618 & 0.618 & -1 \\ 1 & -1.618 & 0.618 & 0.618 & -1.618 & 1 \\ 1 & -2 & 2 & -2 & 2 & -1 \end{pmatrix} \begin{pmatrix} f_0 \\ f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \end{pmatrix} \tag{4.50}$$

and the integral is approximately

$$\int_{-1}^{1} f(x)dx \approx \left(\tfrac{1}{5} \;\; 0 \; -\tfrac{2}{15} \;\; 0 \; -\tfrac{2}{75} \;\; 0 \right) \begin{pmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \end{pmatrix}$$

$$= 0.0400 f_0 + 0.3607 f_1 + 0.5993 f_2 + 0.5993 f_3 + 0.3607 f_4 + 0.0400 f_5. \tag{4.51}$$

Clenshaw Curtis weights of very high order can be calculated efficiently [20, 21] using the FFT algorithm (fast Fourier transformation, Sect. 7.3.2).

4.2.2 Gaussian Integration

Now we will optimize the positions of the N quadrature points x_i to obtain the maximum possible accuracy. We approximate the integral by a sum

$$\int_a^b f(x)dx \approx \sum_{i=1}^{N} f(x_i)w_i \tag{4.52}$$

and determine the $2N$ parameters x_i and w_i such that a polynomial of order $2N-1$ is integrated exactly. This can be achieved with the help of a set of polynomials which are orthogonal with respect to the scalar product

$$< fg >= \int_a^b f(x)g(x)w(x)dx \tag{4.53}$$

where the weight function $w(x)$ and the interval $[a, b]$ determine a particular set of orthogonal polynomials.

4.2.2.1 Gauss–Legendre Integration

Again we restrict the integration interval to $[-1, 1]$ in the following. For integrals with one or two infinite boundaries see Sect. 4.2.2. The simplest choice for the weight function is

$$w(x) = 1. \tag{4.54}$$

An orthogonal system of polynomials on the interval $[-1, 1]$ can be found using the Gram–Schmidt method:

$$P_0 = 1 \tag{4.55}$$

$$P_1 = x - \frac{P_0}{< P_0 P_0 >} \int_{-1}^{1} x P_0(x)dx = x \tag{4.56}$$

$$\begin{aligned} P_2 &= x^2 - \frac{P_1}{< P_1 P_1 >} \int_{-1}^{1} x^2 P_1(x)dx - \frac{P_0}{< P_0 P_0 >} \int_{-1}^{1} x^2 P_0(x)dx \\ &= x^2 - \frac{1}{3} \end{aligned} \tag{4.57}$$

$$P_n = x^n - \frac{P_{n-1}}{< P_{n-1}P_{n-1} >}\int_{-1}^{1} x^n P_{n-1}(x)dx$$
$$-\frac{P_{n-2}}{< P_{n-2}P_{n-2} >}\int_{-1}^{1} x^n P_{n-2}(x)dx - \cdots . \tag{4.58}$$

The P_n are known as Legendre-polynomials. Consider now a polynomial $p(x)$ of order $2N-1$. It can be interpolated at the N quadrature points x_i using the Lagrange method by a polynomial $\widetilde{p}(x)$ of order $N-1$:

$$\widetilde{p}(x) = \sum_{j=1}^{N} L_j(x)p(x_j). \tag{4.59}$$

Then $p(x)$ can be written as

$$p(x) = \widetilde{p}(x) + (x-x_1)(x-x_2)\dots(x-x_N)q(x). \tag{4.60}$$

Obviously $q(x)$ is a polynomial of order $(2N-1)-N = N-1$. Now choose the positions x_i as the roots of the Legendre polynomial of order N

$$(x-x_1)(x-x_2)\dots(x-x_N) = P_N(x). \tag{4.61}$$

Then we have

$$\int_{-1}^{1}(x-x_1)(x-x_2)\dots(x-x_N)q(x)dx = 0 \tag{4.62}$$

since P_N is orthogonal to the polynomial of lower order. But now

$$\int_{-1}^{1} p(x)dx = \int_{-1}^{1}\widetilde{p}(x)dx = \int_{-1}^{1}\sum_{j=1}^{N} p(x_j)L_j(x)dx = \sum_{j=1}^{N} w_j p(x_j) \tag{4.63}$$

with the weight factors

$$w_j = \int_{-1}^{1} L_j(x)dx. \tag{4.64}$$

Example (Gauss–Legendre integration with two quadrature points) The 2nd order Legendre polynomial

$$P_2(x) = x^2 - \frac{1}{3} \tag{4.65}$$

has two roots

$$x_{1,2} = \pm\sqrt{\frac{1}{3}}. \tag{4.66}$$

The Lagrange polynomials are

$$L_1 = \frac{x - \sqrt{\frac{1}{3}}}{-\sqrt{\frac{1}{3}} - \sqrt{\frac{1}{3}}} \quad L_2 = \frac{x + \sqrt{\frac{1}{3}}}{\sqrt{\frac{1}{3}} + \sqrt{\frac{1}{3}}} \tag{4.67}$$

and the weights

$$w_1 = \int_{-1}^{1} L_1 dx = -\frac{\sqrt{3}}{2}\left(\frac{x^2}{2} - \sqrt{\frac{1}{3}}x\right)_{-1}^{1} = 1 \tag{4.68}$$

$$w_2 = \int_{-1}^{1} L_2 dx = \frac{\sqrt{3}}{2}\left(\frac{x^2}{2} + \sqrt{\frac{1}{3}}x\right)_{-1}^{1} = 1. \tag{4.69}$$

This gives the integral rule

$$\int_{-1}^{1} f(x)dx \approx f\left(-\sqrt{\frac{1}{3}}\right) + f\left(\sqrt{\frac{1}{3}}\right). \tag{4.70}$$

For a general integration interval we substitute

$$x = \frac{a+b}{2} + \frac{b-a}{2}u \tag{4.71}$$

and find the approximation

$$\int_a^b f(x)dx = \int_{-1}^{1} f\left(\frac{a+b}{2} + \frac{b-a}{2}u\right)\frac{b-a}{2}du$$

$$\approx \frac{b-a}{2}\left(f\left(\frac{a+b}{2} - \frac{b-a}{2}\sqrt{\frac{1}{3}}\right) + f\left(\frac{a+b}{2} + \frac{b-a}{2}\sqrt{\frac{1}{3}}\right)\right). \tag{4.72}$$

The next higher order Gaussian rule is given by

$$n = 3 : w_1 = w_3 = 5/9,\ w_2 = 8/9,\ x_3 = -x_1 = 0.77459\ldots,\ x_2 = 0. \tag{4.73}$$

4.2.2.2 Other Types of Gaussian Integration

Further integral rules can be obtained by using other sets of orthogonal polynomials, for instance

Chebyshev Polynomials

$$w(x) = \frac{1}{\sqrt{1-x^2}} \tag{4.74}$$

$$\int_{-1}^{1} f(x)dx = \int_{-1}^{1} f(x)\sqrt{1-x^2}w(x)dx \tag{4.75}$$

$$T_{n+1}(x) = 2x\, T_n(x) - T_{n-1}(x) \tag{4.76}$$

$$x_k = \cos\left(\frac{2k-1}{2N}\pi\right) \quad w_k = \frac{\pi}{N}. \tag{4.77}$$

Hermite Polynomials

$$w(x) = e^{-x^2} \tag{4.78}$$

$$\int_{-\infty}^{\infty} f(x)dx = \int_{-\infty}^{\infty} f(x)e^{x^2} w(x)dx \tag{4.79}$$

$$H_0(x) = 1, \quad H_1(x) = 2x, \quad H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x).$$

Laguerre Polynomials

$$w(x) = e^{-x} \tag{4.80}$$

$$\int_{0}^{\infty} f(x)dx = \int_{0}^{\infty} f(x)e^{x} w(x)dx \tag{4.81}$$

$$L_0(x) = 1, \quad L_1(x) = 1-x, \quad L_{n+1}(x) = \frac{1}{n+1}\left((2n+1-x)L_n(x) - nL_{n-1}(x)\right). \tag{4.82}$$

4.2.2.3 Connection with an Eigenvalue Problem

The determination of quadrature points and weights can be formulated as an eigenvalue problem [22, 23]. Any set of orthogonal polynomials $P_n(x)$ with

$$\int_a^b P_m(x)P_n(x)w(x)dx = \delta_{m,n} \tag{4.83}$$

satisfies a three term recurrence relation

$$P_{n+1}(x) = (a_{n+1}x + b_{n+1})\,P_n(x) - c_{n+1}P_{n-1}(x) \tag{4.84}$$

with $a_n > 0$, $c_n > 0$ which can be written in matrix form [24]

$$x\begin{pmatrix} P_0(x) \\ P_1(x) \\ \\ \\ P_{N-1}(x) \end{pmatrix} = \begin{pmatrix} -\frac{b_1}{a_1} & \frac{1}{a_1} & & & & \\ \frac{c_2}{a_2} & -\frac{b_2}{a_2} & \frac{1}{a_2} & & & \\ & \ddots & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & \frac{c_{N-1}}{a_{N-1}} & -\frac{b_{N-1}}{a_{N-1}} & \frac{1}{a_{N-1}} \\ & & & & \frac{c_N}{a_N} & -\frac{b_N}{a_N} \end{pmatrix} \begin{pmatrix} P_0(x) \\ P_1(x) \\ \\ \\ P_{N-1}(x) \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ \vdots \\ \vdots \\ 0 \\ \frac{1}{a_N}P_N(x) \end{pmatrix} \tag{4.85}$$

or shorter

$$x\mathbf{P}(x) = T\mathbf{P}(x) + \frac{1}{a_N}P_N(x)\mathbf{e}_{N-1} \tag{4.86}$$

with a tridiagonal matrix T. Obviously $P_N(x) = 0$ if and only if

$$x_j\mathbf{P}(x_j) = T\mathbf{P}(x_j), \tag{4.87}$$

hence the roots of $P_N(x)$ are given by the eigenvalues of T. The matrix T is symmetric if the polynomials are orthonormal, otherwise it can be transformed into a symmetric tridiagonal matrix by an orthogonal transformation [24]. Finally the quadrature weight corresponding to the eigenvalue x_j can be calculated from the first component of the corresponding eigenvector $\mathbf{u}_j$ [22] as

$$w_j = u_{j,1}^2 \times \int_a^b w(x)dx. \tag{4.88}$$

Problems

Problem 4.1 Romberg Integration

Use the trapezoidal rule

$$T(h) = h\left(\frac{1}{2}f(a) + f(a+h) + \cdots f(b-h) + \frac{1}{2}f(b)\right) = \int_a^b f(x)dx + \cdots \tag{4.89}$$

with the step sequence

$$h_i = \frac{h_0}{2^i} \tag{4.90}$$

and calculate the elements of the triangular matrix

$$T(i,0) = T(h_i) \tag{4.91}$$

$$T(i,k) = T(i+1,k-1) + \frac{T(i,k-1) - T(i+1,k-1)}{1 - \frac{h_i^2}{h_{i+k}^2}} \tag{4.92}$$

to obtain the approximations

$$T_{01} = P_{01}, T_{02} = P_{012}, T_{03} = P_{0123}, \ldots \tag{4.93}$$

- calculate

  $$\int_0^{\pi^2} \sin(x^2)dx = 0.6773089370468890331\ldots \tag{4.94}$$

  and compare the absolute error of the trapezoidal sums $T(h_i) = T_{i,0}$ and the extrapolated values $T_{0,i}$.
- calculate

  $$\int_\varepsilon^1 \frac{dx}{\sqrt{x}} \tag{4.95}$$

  for $\varepsilon = 10^{-3}$. Compare with the composite midpoint rule

  $$T(h) = h\left(f\left(a+\frac{h}{2}\right) + f\left(a+\frac{3h}{2}\right) + \cdots + f\left(b-\frac{3h}{2}\right) + f\left(b-\frac{h}{2}\right)\right) \tag{4.96}$$