10

Numerical integration – II

10.1 Introduction

In Section 7.2 we described the Newton–Cotes family of formulae for numerical integration. These were constructed by replacing the integrand by its Lagrange interpolation polynomial with equally spaced interpolation points and integrating this exactly. Here, we consider another family of numerical integration rules, called Gauss quadrature formulae, which are based on replacing the integrand f by its Hermite interpolation polynomial and choosing the interpolation points x_j in such a way that, after integrating the Hermite polynomial, the derivative values $f'(x_j)$ do not enter the quadrature formula. It turns out that this can be achieved by requiring that the x_j are roots of a polynomial of a certain degree from a system of orthogonal polynomials.

10.2 Construction of Gauss quadrature rules

Suppose that the function f is defined on the closed interval $[a, b]$ and that it is continuous and differentiable on this interval. Suppose, further, that w is a weight function, defined, positive, continuous and integrable on (a, b). We wish to construct quadrature formulae for the approximate evaluation of the integral

$$\int_a^b w(x) f(x) \mathrm{d}x \,.$$

For a nonnegative integer n, let x_i, $i = 0, \ldots, n$, be $n + 1$ points in the interval $[a, b]$; the precise location of these points will be determined later on. The Hermite interpolation polynomial of degree $2n + 1$ for the function f is given by the expression (see Section 6.4)

$$p_{2n+1}(x) = \sum_{k=0}^{n} H_k(x) f(x_k) + \sum_{k=0}^{n} K_k(x) f'(x_k)\,, \tag{10.1}$$

where

$$\begin{aligned} H_k(x) &= [L_k(x)]^2 (1 - 2L_k'(x_k)(x - x_k))\,, \\ K_k(x) &= [L_k(x)]^2 (x - x_k)\,. \end{aligned} \tag{10.2}$$

Further, for $n \geq 1$, $L_k \in \mathcal{P}_n$ is defined by

$$L_k(x) = \prod_{\substack{i=0\\ i\neq k}}^{n} \frac{x - x_i}{x_k - x_i}\,, \qquad k = 0, 1, \ldots, n\,;$$

if $n = 0$, we let $L_0(x) \equiv 1$ and thereby $H_0(x) \equiv 1$ and $K_0(x) = x - x_0$ for this value of n. Thus, we deduce from (10.1) that

$$\begin{aligned} \int_a^b w(x) f(x) \mathrm{d}x &\approx \int_a^b w(x) p_{2n+1}(x) \mathrm{d}x \\ &= \sum_{k=0}^{n} W_k f(x_k) + \sum_{k=0}^{n} V_k f'(x_k)\,, \end{aligned} \tag{10.3}$$

where

$$W_k = \int_a^b w(x) H_k(x) \mathrm{d}x\,, \qquad V_k = \int_a^b w(x) K_k(x) \mathrm{d}x\,.$$

There is an obvious advantage in choosing the points x_k in such a way that all the coefficients V_k are zero, for then the derivative values $f'(x_k)$ are not required. Recalling the form of the polynomial K_k and inserting it into the defining expression for V_k, we have

$$\begin{aligned} V_k &= \int_a^b w(x) [L_k(x)]^2 (x - x_k) \mathrm{d}x \\ &= C_n \int_a^b w(x) \pi_{n+1}(x) L_k(x) \mathrm{d}x\,, \end{aligned} \tag{10.4}$$

where $\pi_{n+1}(x) = (x - x_0) \ldots (x - x_n)$ and

$$C_n = \begin{cases} \left(\prod_{i=0, i\neq k}^{n} (x_k - x_i)^{-1}\right) & \text{if } n \geq 1\,, \\ 1 & \text{if } n = 0\,. \end{cases}$$

Since π_{n+1} is of degree $n + 1$ while $L_k(x)$ is of degree n for each k, $0 \leq k \leq n$, each V_k will be zero if the polynomial π_{n+1} is orthogonal to every polynomial of lower degree with respect to the weight function

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w. We can therefore construct the required quadrature formula (10.3) with $V_k = 0$, $k = 0, \ldots, n$, by choosing the points x_k, $k = 0, \ldots, n$, to be the zeros of the polynomial of degree $n+1$ in a system of orthogonal polynomials over the interval (a, b) with respect to the weight function w; we know from Theorem 9.4 that these zeros are real and distinct, and all lie in the open interval (a, b).

Having chosen the location of the points x_k, we now consider W_k:

$$\begin{aligned} W_k &= \int_a^b w(x) H_k(x) \mathrm{d}x \\ &= \int_a^b w(x) [L_k(x)]^2 (1 - 2L_k'(x_k)(x - x_k)) \mathrm{d}x \\ &= \int_a^b w(x) [L_k(x)]^2 \mathrm{d}x - 2L_k'(x_k) V_k \,. \end{aligned} \tag{10.5}$$

Since $V_k = 0$, the second term in the last line vanishes and thus we obtain the following numerical integration formula, known as the **Gauss quadrature**[1] rule:

$$\int_a^b w(x) f(x) \mathrm{d}x \approx \mathcal{G}_n(f) = \sum_{k=0}^{n} W_k f(x_k) \,, \tag{10.6}$$

where the **quadrature weights** are

$$W_k = \int_a^b w(x) [L_k(x)]^2 \mathrm{d}x \,, \tag{10.7}$$

and the **quadrature points** x_k, $k = 0, \ldots, n$, are chosen as the zeros of the polynomial of degree $n+1$ from a system of orthogonal polynomials over the interval (a, b) with respect to the weight function w. Since this quadrature rule was obtained by exact integration of the Hermite interpolation polynomial of degree $2n+1$ for f, it gives the exact result whenever f is a polynomial of degree $2n+1$ or less.

Example 10.1 *Consider the case* $n = 1$, *with the weight function* $w(x) \equiv 1$ *over the interval* $(0, 1)$.

The quadrature points x_0, x_1 are then the zeros of the polynomial φ_2 constructed in Example 9.5 and given by (9.8),

$$\varphi_2(x) = x^2 - x + \tfrac{1}{6} \,, \tag{10.8}$$

[1] Carl Friedrich Gauss, *Methodus nova integralium valores per approximationem inveniendi*, 1814.

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and therefore

$$x_0 = \tfrac{1}{2} - \sqrt{\tfrac{1}{12}}\,, \quad x_1 = \tfrac{1}{2} + \sqrt{\tfrac{1}{12}}\,.$$

Clearly, x_0 and x_1 belong to the open interval $(0, 1)$, in accordance with Theorem 9.4. The weights are obtained from (10.7):

$$\begin{aligned} W_0 &= \int_0^1 \left(\frac{x - x_1}{x_0 - x_1}\right)^2 \mathrm{d}x \\ &= 3\int_0^1 (x^2 - 2x_1 x + x_1^2)\,\mathrm{d}x \\ &= 3(\tfrac{1}{3} - x_1 + x_1^2) \\ &= \tfrac{1}{2}\,, \end{aligned} \tag{10.9}$$

and $W_1 = \frac{1}{2}$ in the same way. We thus have the Gauss quadrature rule

$$\int_0^1 f(x)\mathrm{d}x \approx \tfrac{1}{2}f(\tfrac{1}{2} - \sqrt{\tfrac{1}{12}}) + \tfrac{1}{2}f(\tfrac{1}{2} + \sqrt{\tfrac{1}{12}})\,, \tag{10.10}$$

which is exact whenever f is a polynomial of degree $2 \times 1 + 1 = 3$ or less. ◇

10.3 Direct construction

The calculation of the weights and the quadrature points in a Gauss quadrature rule requires little work when the system of orthogonal polynomials is already known. If this is not known, at the very least it is necessary to construct the polynomial from the system whose roots are the quadrature points; in that case a straightforward approach, which avoids this construction, may be easier.

Suppose, for example, that we wish to find the values of A_0, A_1, x_0 and x_1 such that the quadrature rule

$$\int_0^1 f(x)\mathrm{d}x \approx A_0 f(x_0) + A_1 f(x_1) \tag{10.11}$$

is exact for all $f \in \mathcal{P}_3$.

We have to determine four unknowns, A_0, A_1, x_0 and x_1, so we need four equations; thus we take, in turn, $f(x) \equiv 1$, $f(x) = x$, $f(x) = x^2$ and $f(x) = x^3$ and demand that the quadrature rule (10.11) is exact (that is, the integral of f is equal to the corresponding approximation obtained by inserting f into the right-hand side of (10.11)). Hence,

$$1 = A_0 + A_1\,, \tag{10.12}$$

$$\begin{aligned}
\tfrac{1}{2} &= A_0x_0 + A_1x_1\,, &(10.13)\\
\tfrac{1}{3} &= A_0x_0^2 + A_1x_1^2\,, &(10.14)\\
\tfrac{1}{4} &= A_0x_0^3 + A_1x_1^3\,. &(10.15)
\end{aligned}$$

It remains to solve this system. To do so, we consider the quadratic polynomial π_2 defined by

$$\pi_2(x) = (x - x_0)(x - x_1)$$

whose roots are the unknown quadrature points x_0 and x_1. In expanded form, $\pi_2(x)$ can be written as

$$\pi_2(x) = x^2 + px + q\,.$$

First we shall determine p and q; then we shall find the roots x_0 and x_1 of π_2. We shall then insert the values of x_0 and x_1 into (10.13) and solve the linear system (10.12), (10.13) for A_0 and A_1.

To find p and q, we multiply (10.12) by q, (10.13) by p and (10.14) by 1, and we add up the resulting equations to deduce that

$$\begin{aligned}
\tfrac{1}{3} + \tfrac{1}{2}p + q &= A_0(x_0^2 + px_0 + q) + A_1(x_1^2 + px_1 + q)\\
&= A_0\pi_2(x_0) + A_1\pi_2(x_1) = A_0 \cdot 0 + A_1 \cdot 0 = 0\,.
\end{aligned}$$

Therefore,

$$\tfrac{1}{3} + \tfrac{1}{2}p + q = 0\,. \tag{10.16}$$

Similarly, we multiply (10.13) by q, (10.14) by p and (10.15) by 1, and we add up the resulting equations to obtain

$$\begin{aligned}
\tfrac{1}{4} + \tfrac{1}{3}p + \tfrac{1}{2}q &= A_0x_0(x_0^2 + px_0 + q) + A_1x_1(x_1^2 + px_1 + q)\\
&= A_0x_0\pi_2(x_0) + A_1x_1\pi_2(x_1) = A_0 \cdot 0 + A_1 \cdot 0 = 0\,.
\end{aligned}$$

Thus,

$$\tfrac{1}{4} + \tfrac{1}{3}p + \tfrac{1}{2}q = 0\,. \tag{10.17}$$

From (10.16) and (10.17) we immediately find that $p = -1$ and $q = \frac{1}{6}$. Having determined p and q, we see that

$$\pi_2(x) = x^2 - x + \tfrac{1}{6}\,,$$

in agreement with (10.8). We then find the roots of this quadratic polynomial to give x_0 and x_1 as before. With these values of x_0 and x_1 we deduce from (10.12) and (10.13) that

$$\begin{aligned}
A_0 + A_1 &= 1\,,\\
A_0(\tfrac{1}{2} + \sqrt{\tfrac{1}{12}}) - A_1(\tfrac{1}{2} - \sqrt{\tfrac{1}{12}}) &= 0\,,
\end{aligned}$$

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and therefore $A_0 = A_1 = \frac{1}{2}$. Thus, we conclude that the required quadrature rule is (10.10), as before.

It is easy to see that equations (10.16) and (10.17) express the condition that the polynomial $x^2 + px + q$ is orthogonal to the polynomials 1 and x respectively. This alternative approach has simply constructed a quadratic polynomial from a system of orthogonal polynomials by requiring that it is orthogonal to every polynomial of lower degree, instead of building up the whole system of orthogonal polynomials.

A straightforward calculation shows that, in general, the quadrature rule (10.10) is not exact for polynomials of degree higher than 3 (take $f(x) = x^4$, for example, to verify this).

Example 10.2 *We shall apply the quadrature rule (10.10) to compute an approximation to the integral* $I = \int_0^1 \mathrm{e}^x \mathrm{d}x$.

Using (10.10) with $f(x) = \exp(x) = \mathrm{e}^x$ yields

$$I \approx \tfrac{1}{2}\exp\left(\tfrac{1}{2} - \sqrt{\tfrac{1}{12}}\right) + \tfrac{1}{2}\exp\left(\tfrac{1}{2} + \sqrt{\tfrac{1}{12}}\right) = \sqrt{\mathrm{e}}\cosh\sqrt{\tfrac{1}{12}}\,.$$

On rounding to six decimal digits, $I \approx 1.717896$. The exact value of the integral is $I = \mathrm{e} - 1 = 1.718282$, rounding to six decimal digits. ◇

10.4 Error estimation for Gauss quadrature

The next theorem provides a bound on the error that has been committed by approximating the integral on the left-hand side of (10.6) by the quadrature rule on the right.

Theorem 10.1 *Suppose that w is a weight function, defined, integrable, continuous and positive on (a, b), and that f is defined and continuous on $[a, b]$; suppose further that f has a continuous derivative of order $2n+2$ on $[a, b]$, $n \geq 0$. Then, there exists a number η in (a, b) such that*

$$\int_a^b w(x)f(x)\mathrm{d}x - \sum_{k=0}^{n} W_k f(x_k) = K_n f^{(2n+2)}(\eta)\,, \tag{10.18}$$

and

$$K_n = \frac{1}{(2n+2)!}\int_a^b w(x)[\pi_{n+1}(x)]^2 \mathrm{d}x\,.$$

Consequently, the integration formula (10.6), (10.7) will give the exact result for every polynomial of degree $2n+1$.

Proof Recalling the definition of the Hermite interpolation polynomial p_{2n+1} for the function f and using Theorem 6.4, we have

$$\begin{aligned}\int_a^b w(x)f(x)\mathrm{d}x - \sum_{k=0}^{n} W_k f(x_k) &= \int_a^b w(x)(f(x) - p_{2n+1}(x))\mathrm{d}x \\ &= \int_a^b w(x)\frac{f^{(2n+2)}(\xi(x))}{(2n+2)!}[\pi_{n+1}(x)]^2\mathrm{d}x\,. \end{aligned} \tag{10.19}$$

However, by the Integral Mean Value Theorem, Theorem A.6, the last term is equal to

$$\frac{f^{(2n+2)}(\eta)}{(2n+2)!}\int_a^b w(x)[\pi_{n+1}(x)]^2\mathrm{d}x\,,$$

for some $\eta \in (a, b)$, and hence the desired error bound. □

Note that, by virtue of Theorem 10.1, the Gauss quadrature rule gives the exact value of the integral when f is a polynomial of degree $2n+1$ or less, which is the highest possible degree that one can hope for with the $2n+2$ free parameters consisting of the quadrature weights W_k, $k = 0, \ldots, n$, and the quadrature points x_k, $k = 0, \ldots, n$.

A different approach leads to a proof of convergence of the Gauss formulae $\mathcal{G}_n(f)$, defined in (10.6), (10.7), as $n \to \infty$.

Theorem 10.2 *Suppose that the weight function w is defined, positive, continuous and integrable on the open interval (a, b). Suppose also that the function f is continuous on the closed interval $[a, b]$. Then,*

$$\lim_{n\to\infty} \mathcal{G}_n(f) = \int_a^b w(x)f(x)\mathrm{d}x\,.$$

Proof If we choose any positive real number ε_0 then, since f is continuous on $[a, b]$, the Weierstrass Theorem (Theorem 8.1) shows that there is a polynomial p such that

$$|f(x) - p(x)| \le \varepsilon_0 \qquad \text{for all } x \in [a, b]\,. \tag{10.20}$$

Let N be the degree of this polynomial, and write p as p_N.

Thus we deduce that

$$\begin{aligned}\int_a^b w(x)f(x)\mathrm{d}x - \mathcal{G}_n(f) &= \int_a^b w(x)[f(x) - p_N(x)]\mathrm{d}x \\ &\quad + \int_a^b w(x)p_N(x)\mathrm{d}x - \mathcal{G}_n(p_N) \\ &\quad + \mathcal{G}_n(p_N) - \mathcal{G}_n(f)\,. \end{aligned} \tag{10.21}$$

Consider the first term on the right of this equality; it follows from (10.20) that

$$\left|\int_a^b w(x)[f(x) - p_n(x)]\mathrm{d}x\right| \leq \varepsilon_0 W\,,$$

where

$$W = \int_a^b w(x)\mathrm{d}x\,.$$

For the last term on the right of (10.21),

$$\begin{aligned} |\mathcal{G}_n(f) - \mathcal{G}_n(p_N)| &\leq \sum_{k=0}^{n} |W_k[f(x_k) - p_N(x_k)]| \\ &\leq \varepsilon_0 \sum_{k=0}^{n} W_k \\ &= \varepsilon_0 \int_a^b w(x)\mathrm{d}x \\ &= \varepsilon_0 W\,, \end{aligned} \tag{10.22}$$

where we have used the fact that all the quadrature weights W_k are positive (see (10.7)), and that a Gauss quadrature rule integrates a constant function exactly. Now for the middle term in (10.21), if we define N_0 to be the integer part of $\frac{1}{2}N$, we see that when $n \geq N_0$ the quadrature formula is exact for all polynomials of degree $2N_0 + 1$ or less, and hence for the polynomial p_N (given that $N \leq 2N_0 + 1 \leq 2n + 1$). Therefore,

$$\int_a^b w(x)p_N(x)\mathrm{d}x - \mathcal{G}_n(p_N) = 0 \quad \text{if } n \geq N_0\,.$$

Putting these three terms together, we see that

$$\left|\int_a^b w(x)f(x)\mathrm{d}x - \mathcal{G}_n(f)\right| \leq \varepsilon_0 W + 0 + \varepsilon_0 W \quad \text{if } n \geq N_0\,.$$

Finally, given any positive number ε, we define $\varepsilon_0 = \varepsilon/(2W)$ and find the corresponding value of $N_0 = N_0(\varepsilon)$ to deduce that

$$\left|\int_a^b w(x)f(x)\mathrm{d}x - \mathcal{G}_n(f)\right| \leq \varepsilon \quad \text{if } n \geq N_0\,,$$

which is what we were required to prove. □

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The interest of this theorem is mainly theoretical, as it gives no indication of how rapidly the error tends to zero. However, it does show the importance of the fact that the weights W_k are positive. Much of the above proof would apply with little change to the Newton–Cotes formulae of Section 7.2. We saw there that for the formulae of order 1 and 2, the trapezium rule and Simpson's rule, the weights are positive. However, when $n > 8$ some of the weights in the Newton–Cotes formula of order n become negative. In this case we have $\sum_{k=0}^{n} W_k = (b-a)$, but we find that $\sum_{k=0}^{n} |W_k| \to \infty$ as $n \to \infty$, so the proof breaks down. Stronger conditions must be imposed on the function f to ensure that the Newton–Cotes formula converges to the required integral. (See the example in Section 7.4.)

10.5 Composite Gauss formulae

It is often useful to define composite Gauss formulae, just as we did for the trapezium rule and Simpson's rule in Section 7.5. Let us suppose, for the sake of simplicity, that $w(x) \equiv 1$. We divide the range $[a, b]$ into m subintervals $[x_{j-1}, x_j]$, $j = 1, 2, \ldots, m$, $m \geq 2$, each of width $h = (b-a)/m$, and write

$$\int_a^b f(x)\mathrm{d}x = \sum_{j=1}^{m} \int_{x_{j-1}}^{x_j} f(x)\mathrm{d}x \,,$$

where

$$x_j = a + jh \,, \qquad j = 0, 1, \ldots, m \,.$$

We then map each of the subintervals $[x_{j-1}, x_j]$, $j = 1, 2, \ldots, m$, onto the reference interval $[-1, 1]$ by the change of variable

$$x = \tfrac{1}{2}(x_{j-1} + x_j) + \tfrac{1}{2}ht \,, \qquad t \in [-1, 1] \,,$$

giving

$$\int_a^b f(x)\mathrm{d}x = \tfrac{1}{2}h \sum_{j=1}^{m} \int_{-1}^{1} g_j(t)\mathrm{d}t = \tfrac{1}{2}h \sum_{j=1}^{m} I_j \,,$$

where

$$g_j(t) = f\left(\tfrac{1}{2}(x_{j-1} + x_j) + \tfrac{1}{2}ht\right) \quad \text{and} \quad I_j = \int_{-1}^{1} g_j(t)\mathrm{d}t \,.$$

The composite Gauss quadrature rule is then obtained by applying the same Gauss formula to each of the integrals I_j. This gives

$$\begin{aligned}\int_a^b f(x)\mathrm{d}x &\approx \tfrac{1}{2}h\sum_{j=1}^{m}\sum_{k=0}^{n} W_k g_j(\xi_k) \\ &= \tfrac{1}{2}h\sum_{j=1}^{m}\sum_{k=0}^{n} W_k f\left(\tfrac{1}{2}\left(x_{j-1}+x_j\right)+\tfrac{1}{2}h\xi_k\right),\end{aligned} \tag{10.23}$$

where ξ_k are the quadrature points in $(-1,1)$ and W_k are the associated weights for $k=0,\ldots,n$ with $n\geq 0$.

An expression for the error of this composite formula is obtained, as in Section 7.5, by adding the expressions (10.18) for the errors in the integrals I_j. The result is

$$\mathcal{E}_{n,m} = C_n \frac{(b-a)^{2n+3}}{2^{2n+3}m^{2n+2}(2n+2)!} f^{(2n+2)}(\eta) \tag{10.24}$$

where $\eta \in (a,b)$ and

$$C_n = \int_{-1}^{1} [\pi_{n+1}(t)]^2 \mathrm{d}t\,.$$

Definition 10.1 *The* **composite midpoint rule** *is the composite Gauss formula with $w(x)\equiv 1$ and $n=0$ defined by*

$$\int_a^b f(x)\mathrm{d}x \approx h\sum_{j=1}^{m} f(a+(j-\tfrac{1}{2})h)\,. \tag{10.25}$$

This follows from the fact that when $n=0$ there is one quadrature point $\xi_0=0$ in $(-1,1)$, which is at the midpoint of the interval, and the corresponding quadrature weight W_0 is equal to the length of the interval $(-1,1)$, *i.e.*, $W_0=2$. It follows from (10.24) with $n=0$ and

$$C_0 = \int_{-1}^{1} t^2\mathrm{d}t = \tfrac{2}{3}$$

that the error in the composite midpoint rule is

$$\mathcal{E}_{0,m} = \frac{(b-a)^3}{24m^2} f''(\eta)\,,$$

where $\eta\in(a,b)$, provided that the function f has a continuous second derivative on $[a,b]$.

10.6 Radau and Lobatto quadrature

We have now discussed two types of quadrature formulae, which have the same form, $\sum_{k=0}^{n} W_k f(x_k)$. In the Newton–Cotes formulae the (equally spaced) quadrature points x_k are given, and we were able to find the weights W_k so that the result was exact for polynomials of degree n. By allowing the quadrature points as well as the weights to be freely chosen, we constructed Gauss quadrature formulae which were exact for polynomials of degree $2n+1$. There are also many possible formulae of mixed type, where some, but not all, of the quadrature points are given, and the rest can be freely chosen. We might expect that each quadrature point which is fixed will reduce the degree of polynomial for which such a formula is exact by 1, from the maximum degree of $2n+1$.

It is often useful to be able to fix one of the endpoints of the interval as one of the quadrature points. As an example, suppose we prescribe that $x_0 = a$. Let p_{2n} be an arbitrary polynomial of degree $2n$, and write

$$p_{2n}(x) = (x-a)q_{2n-1}(x) + r\,,$$

where the quotient q_{2n-1} is a polynomial of degree $2n-1$ and the remainder r is a constant. The integral of $w\,p_{2n}$ is then

$$\int_a^b w(x)p_{2n}(x)\mathrm{d}x = \int_a^b (x-a)w(x)q_{2n-1}(x)\mathrm{d}x + r\int_a^b w(x)\mathrm{d}x\,.$$

We can now construct the usual Gauss quadrature formula for the interval $[a,b]$ with the modified weight function $(x-a)w(x)$, giving n quadrature points and n weights $x_k^*,\ W_k^*,\ k=1,\ldots,n$. This formula will be exact for all polynomials q of degree $2n-1$. Provided that the weight function w satisfies the standard conditions on (a,b), the modified weight function does also; in particular it is clearly positive on (a,b). This gives

$$\begin{aligned}\int_a^b w(x)p_{2n}(x)\mathrm{d}x &= \sum_{k=1}^{n} W_k^* q_{2n-1}(x_k^*) + r\int_a^b w(x)\mathrm{d}x \\ &= \sum_{k=1}^{n} \frac{W_k^*}{x_k^*-a} p_{2n}(x_k^*) \\ &\quad + r\left[\int_a^b w(x)\mathrm{d}x - \sum_{k=1}^{n}\frac{W_k^*}{x_k^*-a}\right]. \qquad (10.26)\end{aligned}$$

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The fact that $r = p_{2n}(a)$ then leads us to consider the quadrature rule

$$\int_a^b w(x)f(x)\mathrm{d}x \approx W_0 f(a) + \sum_{k=1}^{n} W_k f(x_k)\,, \tag{10.27}$$

where

$$\begin{aligned} W_k &= W_k^*/(x_k^* - a)\,, \quad k = 1, \ldots, n\,, \\ W_0 &= \int_a^b w(x)\mathrm{d}x - \sum_{k=1}^{n} W_k\,. \end{aligned} \tag{10.28}$$

By construction, this formula is exact for all polynomials of degree $2n$. It is obvious that $W_k > 0$ for $k = 1, \ldots, n$. We leave it as an exercise to show that $W_0 > 0$ also (see Exercise 5).

With only trivial changes it is easy to see how to construct a similar formula where instead of fixing $x_0 = a$ we fix $x_n = b$. These are known as **Radau quadrature formulae**. We leave it as an exercise to construct the formula corresponding to fixing both $x_0 = a$ and $x_n = b$, which is known as a **Lobatto quadrature formula**; as might be expected, this is exact for all polynomials of degree $2n - 1$ (see Exercise 7).

The formal process could evidently be generalised to allow for fixing one of the quadrature points at an internal point c, where $a < c < b$. However, this leads to the difficulty that the modified weight function

$$w^*\colon x \mapsto (x - c)w(x)$$

is not positive over the whole interval (a, b); hence we can no longer be sure that it is possible to construct a system of orthogonal polynomials, or, even if we can, that these polynomials will have all their zeros real and distinct and lying in $[a, b]$. In general, therefore, such quadrature formulae may not exist.

10.7 Note

For a detailed guide to the literature on Gauss quadrature rules and its connection to the theory of orthogonal polynomials, we refer to the books cited in the Notes at the end of Chapter 7.

Exercises

10.1 Determine the quadrature points and weights for the weight function $w\colon x \mapsto -\ln x$ on the interval $(0, 1)$, for $n = 0$ and $n = 1$.

10.2 The weights in the Gauss quadrature formula are given by (10.7), which is

$$W_k = \int_a^b w(x)[L_k(x)]^2 \mathrm{d}x\,.$$

Show that W_k can also be calculated from

$$W_k = \int_a^b w(x) L_k(x) \mathrm{d}x\,.$$

(This is a simpler way of calculating W_k than (10.7); the importance of (10.7) is that it shows that the weights are all positive.)

10.3 Suppose that f has a continuous second derivative on $[0,1]$. Show that there is a point ξ in $(0,1)$ such that

$$\int_0^1 x f(x)\mathrm{d}x = \tfrac{1}{2} f(\tfrac{2}{3}) + \tfrac{1}{72} f''(\xi)\,.$$

10.4 Let $n \geq 0$. Write down the quadrature points x_j, $j = 0, \dots, n$, for the weight function $w\colon x \mapsto (1-x^2)^{-1/2}$ on the interval $(-1,1)$.

By induction, or otherwise, show that for positive integer values of n,

$$\sum_{j=0}^{n} \cos(2j+1)\vartheta = \frac{\sin(2n+2)\vartheta}{2\sin\vartheta}\,,$$

unless ϑ is a multiple of π. What is the value of the sum when ϑ is a multiple of π?

Deduce that

$$\sum_{j=0}^{n} T_k(x_j) = \int_{-1}^{1} (1-x^2)^{-1/2} T_k(x)\,\mathrm{d}x\,, \qquad k = 1, \dots, n\,,$$

and show that

$$\sum_{j=0}^{n} T_0(x_j) = \frac{n+1}{\pi} \int_{-1}^{1} (1-x^2)^{-1/2} T_0(x)\,\mathrm{d}x\,,$$

where T_n is the Chebyshev polynomial of degree n.

Deduce that the weights of the quadrature formula with weight function $w\colon x \mapsto (1-x^2)^{-1/2}$ on the interval $(-1,1)$ are

$$W_k = \frac{\pi}{n+1}\,, \qquad k = 0, \dots, n\,.$$

10.5 In the notation for the construction of the Radau quadrature formula in Section 10.6, show that $W_0 > 0$.

10.6 The **Laguerre polynomials**[1] L_j, $j = 0, 1, 2, \ldots$, are the orthogonal polynomials associated with the weight function $w\colon x \mapsto \mathrm{e}^{-x}$ on the semi-infinite interval $(0, \infty)$, with L_j of exact degree j. (See Exercise 5.9.) Show that

$$\int_0^\infty \mathrm{e}^{-x} x[L_j(x) - L_j'(x)]p_r(x)\mathrm{d}x = 0$$

when p_r is any polynomial of degree less than j.

In the Radau formula

$$\int_0^\infty \mathrm{e}^{-x} p_{2n}(x)\mathrm{d}x = W_0 p_{2n}(0) + \sum_{k=1}^{n} W_k p_{2n}(x_k)\,,$$

where one of the quadrature points is fixed at $x = 0$, show that the other quadrature points x_k, $k = 1, \ldots, n$, are the zeros of the polynomial $L_n - L_n'$. Deduce that

$$\int_0^\infty \mathrm{e}^{-x} p_2(x)\mathrm{d}x = \tfrac{1}{2}p_2(0) + \tfrac{1}{2}p_2(2)\,.$$

10.7 Let $n \geq 2$. Show that a polynomial p_{2n-1} of degree $2n-1$ can be written

$$p_{2n-1}(x) = (x-a)(b-x)q_{2n-3}(x) + r(x-a) + s(b-x)\,,$$

where q_{2n-3} is a polynomial of degree $2n-3$, and r and s are constants. Hence construct the Lobatto quadrature formula

$$\int_a^b w(x)f(x)\mathrm{d}x \approx W_0 f(a) + \sum_{k=1}^{n-1} W_k f(x_k) + W_n f(b)\,,$$

which is exact when f is any polynomial of degree $2n-1$. Show that all the weights W_k, $k = 0, 1, \ldots, n$, are positive.

10.8 Construct the Lobatto quadrature formula

$$\int_{-1}^{1} f(x) \approx A_0 f(-1) + A_1 f(x_1) + A_2 f(1)$$

for the interval $(-1, 1)$ with weight function $w(x) \equiv 1$, and with $n = 2$; write down and solve four equations to determine x_1, A_0, A_1 and A_2.

[1] Edmond Nicolas Laguerre (9 April 1834, Bar-le-Duc, France – 14 Aug 1886, Bar-le-Duc, France.)

10.9 Write T_m for the composite trapezium rule (7.15), S_m for the composite Simpson rule (7.17) and M_m for the composite midpoint rule (10.25), each with m subintervals. Show that

$$M_m = 2I_{2m} - I_m\,, \quad S_m = \frac{4I_{2m} - I_m}{3}\,, \quad S_m = \frac{2M_m + I_m}{3}\,.$$