

Chapter 7

Numerical Integration

Definition 7.1. A *weighted quadrature formula* $I_n(f)$ for a function $f \in L[a, b]$ is a formula

$$I_n(f) := \sum_{k=1}^n w_k f(x_k) \quad (7.1)$$

that approximates the definite integral of f on $[a, b]$

$$I(f) := \int_a^b f(x) \rho(x) dx, \quad (7.2)$$

where the weight function $\rho \in L[a, b]$ satisfies $\forall x \in (a, b)$, $\rho(x) > 0$. The points x_k 's at which the integrand f is evaluated are called *nodes* or *abscissa*, and the multiplier w_k 's are called *weights* or *coefficients*.

Example 7.1. If a and/or b are infinite, $I(f)$ and $I_n(f)$ in (7.1) may still be well defined if the *moment of weight function*

$$\mu_j := \int_a^b x^j \rho(x) dx \quad (7.3)$$

exists and is finite for all $j \in \mathbb{N}$.

7.1 Accuracy and convergence

Definition 7.2. The *remainder*, or *error*, of $I_n(f)$ is

$$E_n(f) := I(f) - I_n(f). \quad (7.4)$$

$I_n(f)$ is said to be *convergent* for $\mathcal{C}[a, b]$ iff

$$\forall f \in \mathcal{C}[a, b], \quad \lim_{n \rightarrow +\infty} I_n(f) = I(f). \quad (7.5)$$

Definition 7.3. A subset $\mathbb{V} \subset \mathcal{C}[a, b]$ is *dense* in $\mathcal{C}[a, b]$ iff

$$\forall f \in \mathcal{C}[a, b], \forall \epsilon > 0, \exists f_\epsilon \in \mathbb{V}, \text{ s.t. } \max_{x \in [a, b]} |f(x) - f_\epsilon(x)| \leq \epsilon. \quad (7.6)$$

Theorem 7.4 (Weierstrass). The set of polynomials is dense in $\mathcal{C}[a, b]$. In other words, for any given $f(x) \in \mathcal{C}[a, b]$ and given $\epsilon > 0$, one can find a polynomial $p_n(x)$ (of sufficiently high degree) such that

$$\forall x \in [a, b], \quad |f(x) - p_n(x)| \leq \epsilon. \quad (7.7)$$

Proof. Not required. \square

Theorem 7.5. Let $\{I_n(f) : n \in \mathbb{N}^+\}$ be a sequence of quadrature formulas that approximate $I(f)$, where I_n and $I(f)$ are defined in (7.1). Let \mathbb{V} be a dense subset of $\mathcal{C}[a, b]$. $I_n(f)$ is convergent for $\mathcal{C}[a, b]$ if and only if

- (a) $\forall f \in \mathbb{V}, \lim_{n \rightarrow +\infty} I_n(f) = I(f)$,
- (b) $B := \sup_{n \in \mathbb{N}^+} \sum_{k=1}^n |w_k| < +\infty$.

Proof. For necessity, it is trivial to deduce (a) from (7.5). In contrast, it is highly nontrivial to deduce (b) from (7.5). This is an example of the principle of uniform boundedness, the proof of which is out of scope of this course. See a standard text on functional analysis, e.g. [Cryer, 1982, p. 121].

For the sufficiency, find $f_\epsilon \in \mathbb{V}$ such that (7.6) holds, define $K := \max_{x \in [a, b]} |f(x) - f_\epsilon(x)|$. Then we have

$$\begin{aligned} |E_n(f)| &\leq |I(f) - I(f_\epsilon)| + |I(f_\epsilon) - I_n(f_\epsilon)| + |I_n(f_\epsilon) - I_n(f)| \\ &= \left| \int_a^b [f(x) - f_\epsilon(x)] \rho(x) dx \right| \\ &\quad + |I(f_\epsilon) - I_n(f_\epsilon)| + \left| \sum_{k=1}^n w_k [f(x_k) - f_\epsilon(x_k)] \right| \\ &\leq K \left[\int_a^b \rho(x) dx + \sum_{k=1}^n |w_k| \right] + |I(f_\epsilon) - I_n(f_\epsilon)|, \end{aligned}$$

where the first step follows from the triangular inequality, the second from Definition 7.1, and the third from the integral mean value theorem 0.56. The terms inside the brackets is bounded because of $\rho \in L[a, b]$ and condition (b). By condition (a), $|I(f_\epsilon) - I_n(f_\epsilon)|$ can be made arbitrarily small. The proof is completed by the fact that K can also be arbitrarily small. \square

Definition 7.6. A weighted quadrature formula (7.1) has (polynomial) *degree of exactness* d_E iff

$$\begin{cases} \forall f \in \mathbb{P}_{d_E}, & E_n(f) = 0, \\ \exists g \in \mathbb{P}_{d_E+1}, \text{ s.t. } & E_n(g) \neq 0. \end{cases} \quad (7.8)$$

Lemma 7.7. Let x_1, \dots, x_n be given as distinct nodes of $I_n(f)$. If $d_E \geq n - 1$, then its weights can be deduced as

$$\forall k = 1, \dots, n, \quad w_k = \int_a^b \rho(x) \ell_k(x) dx, \quad (7.9)$$

where $\ell_k(x)$ is the fundamental polynomial for pointwise interpolation in (3.9) applied to the given nodes,

$$\ell_k(x) := \prod_{i \neq k; i=1}^n \frac{x - x_i}{x_k - x_i}. \quad (7.10)$$

Proof. Let $p_{n-1}(f; x)$ be the unique polynomial that interpolates f at the distinct nodes, as in Theorem 3.4. Then

$$\begin{aligned} \sum_{k=1}^n w_k p_{n-1}(x_k) &= \int_a^b p_{n-1}(f; x) \rho(x) dx \\ &= \int_a^b \sum_{k=1}^n \{\ell_k(x) f(x_k)\} \rho(x) dx = \sum_{k=1}^n w_k f(x_k), \end{aligned}$$

where the first step follows from $d_E \geq n-1$ and the second step from the interpolation conditions (3.4), the Lagrange formula, and the uniqueness of $p_{n-1}(f; x)$. The proof is completed by setting f to be the hat function $\hat{B}_k(x)$ (see Definition 4.16) for each x_k . \square

7.2 Newton-Cotes formulas

Definition 7.8. A *Newton-Cotes formula* is a formula (7.1) based on approximating $f(x)$ by interpolating it on uniformly spaced nodes $x_1, \dots, x_n \in [a, b]$.

Definition 7.9. The *trapezoidal rule* is a formula (7.1) based on approximating $f(x)$ by the straight line that connects $(a, f(a))^T$ and $(b, f(b))^T$. In particular, for $\rho(x) \equiv 1$, it is simply

$$I^T(f) = \frac{b-a}{2} [f(a) + f(b)]. \quad (7.11)$$

Example 7.2. Derive the trapezoidal rule for the weight function $\rho(x) = x^{-1/2}$ on the interval $[0, 1]$. Note that one cannot apply (7.11) to $\rho(x)f(x)$ because $\rho(0) = \infty$. (7.9) yields

$$\begin{aligned} w_1 &= \int_0^1 x^{-1/2} (1-x) dx = \frac{4}{3}, \\ w_2 &= \int_0^1 x^{-1/2} x dx = \frac{2}{3}. \end{aligned}$$

Hence the formula is

$$I^T(f) = \frac{2}{3} [2f(0) + f(1)]. \quad (7.12)$$

Theorem 7.10. For $f \in \mathcal{C}^2[a, b]$ with weight function $\rho(x) \equiv 1$, the remainder of the trapezoidal rule satisfies

$$\exists \zeta \in [a, b] \text{ s.t. } E^T(f) = -\frac{(b-a)^3}{12} f''(\zeta). \quad (7.13)$$

Proof. By Theorem 3.4, the interpolating polynomial $p_1(f; x)$ is unique. Then we have

$$\begin{aligned} E^T(f) &= -\int_a^b \frac{f''(\xi(x))}{2} (x-a)(b-x) dx \\ &= -\frac{f''(\zeta)}{2} \int_a^b (x-a)(b-x) dx = -\frac{(b-a)^3}{12} f''(\zeta), \end{aligned}$$

where the first step follows from Theorem 3.6 and the second step from the integral mean value theorem (Theorem 0.56). Here we can apply Theorem 0.56 because

$$w(x) = (x-a)(b-x)$$

is always positive on (a, b) . Also note that ξ is a function of x while ζ is a constant depending only on f , a , and b . \square

Definition 7.11. *Simpson's rule* is a formula (7.1) based on approximating $f(x)$ by a quadratic polynomial that goes through $(a, f(a))^T$, $(b, f(b))^T$, and $(\frac{a+b}{2}, f(\frac{a+b}{2}))^T$. For $\rho(x) \equiv 1$, it is simply

$$I^S(f) = \frac{b-a}{6} \left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right]. \quad (7.14)$$

Theorem 7.12. For $f \in \mathcal{C}^4[a, b]$ with weight function $\rho(x) \equiv 1$, the remainder of Simpson's rule satisfies

$$\exists \zeta \in [a, b] \text{ s.t. } E^S(f) = -\frac{(b-a)^5}{2880} f^{(4)}(\zeta). \quad (7.15)$$

Proof. It is difficult to imitate the proof of Theorem 7.10, since $(x-a)(x-b)(x-\frac{a+b}{2})$ changes sign over $[a, b]$ and the integral mean value theorem is not applicable. To overcome this difficulty, we can formulate the interpolation via a Hermite problem so that Theorem 0.56 can be applied. See problem I in Section 7.5 for the main steps. \square

Example 7.3. Consider the integral

$$I = \int_{-4}^4 \frac{dx}{1+x^2} = 2 \tan^{-1}(4) = 2.6516 \dots \quad (7.16)$$

As shown below, the Newton-Cotes formula appears to be non-convergent.

$n-1$	2	4	6	8	10
I_{n-1}	5.4902	2.2776	3.3288	1.9411	3.5956

Note $n-1$ is the number of sub-intervals that partition $[a, b]$ in Definition 7.8.

7.3 Composite formulas

Definition 7.13. The *composite trapezoidal rule* for approximating $I(f)$ in (7.2) with $\rho(x) \equiv 1$ is

$$I_n^T(f) = \frac{h}{2} f(x_0) + h \sum_{k=1}^{n-1} f(x_k) + \frac{h}{2} f(x_n), \quad (7.17)$$

where $h = \frac{b-a}{n}$ and $x_k = a + kh$.

Theorem 7.14. For $f \in \mathcal{C}^2[a, b]$, the remainder of the composite trapezoidal rule satisfies

$$\exists \xi \in (a, b) \text{ s.t. } E_n^T(f) = -\frac{b-a}{12} h^2 f''(\xi). \quad (7.18)$$

Proof. Apply Theorem 7.10 to the subintervals, sum up the errors, and we have

$$E_n^T(f) = -\frac{b-a}{12} h^2 \left[\frac{1}{n} \sum_{k=0}^{n-1} f''(\xi_k) \right]. \quad (7.19)$$

$f \in \mathcal{C}^2[a, b]$ implies $f'' \in \mathcal{C}[a, b]$. The proof is completed by (7.19) and the intermediate value Theorem 0.32. \square

Definition 7.15. The *composite Simpson's rule* for approximating $I(f)$ in (7.2) with $\rho(x) \equiv 1$ is

$$I_n^S(f) = \frac{h}{3} [f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + \cdots + 4f(x_{n-1}) + f(x_n)], \quad (7.20)$$

where $h = \frac{b-a}{n}$, $x_k = a + kh$, and n is even.

Theorem 7.16. For $f \in C^4[a, b]$ and $n \in 2\mathbb{N}^+$, the remainder of the composite Simpson's rule satisfies

$$\exists \xi \in (a, b) \text{ s.t. } E_n^S(f) = -\frac{b-a}{180} h^4 f^{(4)}(\xi). \quad (7.21)$$

Proof. Exercise. \square

7.4 Gauss formulas

Lemma 7.17. Let $n, m \in \mathbb{N}^+$ and $m \leq n$. Given polynomials $p = \sum_{i=0}^{n+m} p_i x^i \in \mathbb{P}_{n+m}$ and $s = \sum_{i=0}^n s_i x^i \in \mathbb{P}_n$ satisfying $p_{n+m} \neq 0$ and $s_n \neq 0$, there exist unique polynomials $q \in \mathbb{P}_m$ and $r \in \mathbb{P}_{n-1}$ such that

$$p = qs + r. \quad (7.22)$$

Proof. Rewrite (7.22) as

$$\sum_{i=0}^{n+m} p_i x^i = \left(\sum_{i=0}^m q_i x^i \right) \left(\sum_{i=0}^n s_i x^i \right) + \sum_{i=0}^{n-1} r_i x^i. \quad (7.23)$$

Since monomials are linearly independent, (7.23) consists of $n+m+1$ equations, the last $m+1$ of which are

$$\begin{aligned} p_{n+m} &= q_m s_n, \\ p_{n+m-1} &= q_m s_{n-1} + q_{m-1} s_n, \\ &\dots \\ p_n &= q_m s_{n-m} + \dots + q_0 s_n. \end{aligned}$$

This is a nonsingular triangular linear system in terms of the coefficients of q , which can be determined uniquely from coefficients of p and s . Then r can be determined uniquely by $p - qs$ from (7.23). \square

Definition 7.18. The *node polynomial* associated with the nodes x_k 's of a weighted quadrature formula is

$$v_n(x) = \prod_{k=1}^n (x - x_k). \quad (7.24)$$

Theorem 7.19. Suppose a quadrature formula (7.1) has $d_E \geq n-1$. Then it can be improved to have $d_E \geq n+j-1$ where $j \in (0, n]$ by and only by imposing the additional conditions on its node polynomial and weight function,

$$\forall p \in \mathbb{P}_{j-1}, \quad \int_a^b v_n(x) p(x) \rho(x) dx = 0. \quad (7.25)$$

Proof. For the necessity, we have

$$\int_a^b v_n(x) p(x) \rho(x) dx = \sum_{k=1}^n w_k v_n(x_k) p(x_k) = 0,$$

where the first step follows from $d_E \geq n+j-1$ and $v_n(x)p(x) \in \mathbb{P}_{n+j-1}$, and the second step from (7.24).

To prove the sufficiency, we must show that $E_n(p) = 0$ for any $p \in \mathbb{P}_{n+j-1}$. Lemma 7.17 yields

$$\forall p \in \mathbb{P}_{n+j-1}, \exists q \in \mathbb{P}_{j-1}, r \in \mathbb{P}_{n-1}, \text{ s.t. } p = qv_n + r. \quad (7.26)$$

Consequently, we have

$$\begin{aligned} \int_a^b p(x) \rho(x) dx &= \int_a^b q(x) v_n(x) \rho(x) dx + \int_a^b r(x) \rho(x) dx \\ &= \int_a^b r(x) \rho(x) dx = \sum_{k=1}^n w_k r(x_k) \\ &= \sum_{k=1}^n w_k [p(x_k) - q(x_k) v_n(x_k)] = \sum_{k=1}^n w_k p(x_k), \end{aligned}$$

where the first step follows from (7.26), the second from (7.25), the third from the condition of $d_E \geq n-1$, the fourth from (7.26), and the last from (7.24). \square

Definition 7.20. A *Gaussian quadrature formula* is a formula (7.1) whose nodes are the zeros of the polynomial $v_n(x)$ in (7.24) that satisfies (7.25) for $j = n$.

Corollary 7.21. A Gauss formula has $d_E = 2n-1$.

Proof. The index j in (7.25) cannot be $n+1$ because the node polynomial $v_n(x) \in \mathbb{P}_n$ cannot be orthogonal to itself. Therefore we know that $j = n$ in Theorem 7.19 is optimal: the formula (7.1) achieves the highest degree of exactness $2n-1$. From an algebraic viewpoint, the $2n$ degrees of freedom of nodes and weights in (7.1) determine a polynomial of degree at most $2n-1$. The rest follows from Theorem 7.19. \square

Corollary 7.22. Weights of a Gauss formula $I_n(f)$ are

$$\forall k = 1, \dots, n, \quad w_k = \int_a^b \frac{v_n(x)}{(x - x_k) v_n'(x_k)} \rho(x) dx, \quad (7.27)$$

where $v_n(x)$ is the node polynomial that defines $I_n(f)$.

Proof. This follows from Lemma 7.7; also see (3.11). \square

Example 7.4. Derive the Gauss formula of $n = 2$ for the weight function $\rho(x) = x^{-1/2}$ on the interval $[0, 1]$.

We first construct an orthogonal polynomial

$$\pi(x) = c_0 - c_1 x + x^2$$

such that

$$\forall p \in \mathbb{P}_1, \quad \langle p(x), \pi(x) \rangle := \int_0^1 p(x) \pi(x) \rho(x) dx = 0,$$

which is equivalent to $\langle 1, \pi(x) \rangle = 0$ and $\langle x, \pi(x) \rangle = 0$ because $\mathbb{P}_1 = \text{span}(1, x)$. These two conditions yield

$$\begin{aligned} \int_0^1 (c_0 - c_1 x + x^2) x^{-1/2} dx &= \frac{2}{5} + 2c_0 - \frac{2}{3}c_1 = 0, \\ \int_0^1 x(c_0 - c_1 x + x^2) x^{-1/2} dx &= \frac{2}{7} + \frac{2}{3}c_0 - \frac{2}{5}c_1 = 0. \end{aligned}$$

Hence $c_1 = \frac{6}{7}$, $c_0 = \frac{3}{35}$, and the orthogonal polynomial is

$$\pi(x) = \frac{3}{35} - \frac{6}{7}x + x^2$$

with its zeros at

$$x_1 = \frac{1}{7} \left(3 - 2\sqrt{\frac{6}{5}} \right), \quad x_2 = \frac{1}{7} \left(3 + 2\sqrt{\frac{6}{5}} \right).$$

To calculate w_1 and w_2 , we could again use (7.9), but it is simpler to set up a linear system of equations by exploiting Corollary 7.21, i.e. Gauss quadrature is exactly for all constants and linear polynomials,

$$\begin{aligned} w_1 + w_2 &= \int_0^1 x^{-1/2} dx = 2, \\ x_1 w_1 + x_2 w_2 &= \int_0^1 x x^{-1/2} dx = \frac{2}{3}, \end{aligned}$$

which yields

$$w_1 = \frac{-2x_2 + \frac{2}{3}}{x_1 - x_2}, \quad w_2 = \frac{2x_1 - \frac{2}{3}}{x_1 - x_2}.$$

The desired two-point Gauss formula is thus

$$\begin{aligned} I_2^G(f) &= \left(1 + \frac{1}{3}\sqrt{\frac{5}{6}} \right) f \left(\frac{3}{7} - \frac{2}{7}\sqrt{\frac{6}{5}} \right) \\ &\quad + \left(1 - \frac{1}{3}\sqrt{\frac{5}{6}} \right) f \left(\frac{3}{7} + \frac{2}{7}\sqrt{\frac{6}{5}} \right). \end{aligned} \quad (7.28)$$

Theorem 7.23. Each zero of a real orthogonal polynomial over $[a, b]$ is real, simple, and inside (a, b) .

Proof. For fixed $n \geq 1$, suppose $p_n(x)$ does not change sign in $[a, b]$. Then $\int_a^b \rho(x) p_n(x) dx = \langle p_n, p_0 \rangle \neq 0$. But this contradicts orthogonality. Hence there exists $x_1 \in [a, b]$ such that $p_n(x_1) = 0$.

Suppose there were a zero at x_1 which is multiple. Then $\frac{p_n(x)}{(x-x_1)^2}$ would be a polynomial of degree $n-2$. Hence $0 = \langle p_n(x), \frac{p_n(x)}{(x-x_1)^2} \rangle = \langle 1, \frac{p_n^2(x)}{(x-x_1)^2} \rangle > 0$, which is false. Therefore every zero is simple.

Suppose that only $j < n$ zeros of p_n , say x_1, x_2, \dots, x_j , are inside (a, b) and all other zeros are out of (a, b) . Let $v_j(x) = \prod_{i=1}^j (x - x_i) \in \mathbb{P}_j$. Then $p_n v_j = P_{n-j} v_j^2$ where P_{n-j} is a polynomial of degree $n-j$ that does not change sign on $[a, b]$. Hence $|\langle P_{n-j}, v_j^2 \rangle| > 0$, which contradicts the orthogonality of $p_n(x)$ and $v_j(x)$. \square

Corollary 7.24. All nodes of a Gauss formula are real, distinct, and contained in (a, b) .

Proof. This follows from Definition 7.20 and Theorem 7.23. \square

Lemma 7.25. Gauss formulas have positive weights.

Proof. For each $j = 1, 2, \dots, n$, the definition of $\ell_j(x)$ in (7.9) implies $\ell_j^2 \in \mathbb{P}_{2n-2}$, then we have

$$w_j = \sum_{k=1}^n w_k \ell_j^2(x_k) = \int_a^b \rho(x) \ell_j^2(x) dx > 0,$$

where the second step follows from $d_E = 2n-1$ and the last step from the conditions on ρ . \square

Lemma 7.26. A Gauss formula satisfies

$$\sum_{k=1}^n w_k = \mu_0 \in (0, +\infty).$$

Proof. This follows from setting $j = 0$ in (7.3) and applying the condition on ρ in Definition 7.1. \square

Theorem 7.27. Gauss formulas are convergent for $\mathcal{C}[a, b]$.

Proof. Denote by \mathbb{P} the set of real polynomials. Theorem 7.4 states that \mathbb{P} is dense in $\mathcal{C}[a, b]$, i.e. condition (a) in Theorem 7.5 holds. Condition (b) also holds because of Lemma 7.26, (7.3), and $\rho \in L[a, b]$. The rest of the proof follows from Theorem 7.5. \square

Theorem 7.28. For $f \in \mathcal{C}^{2n}[a, b]$, the remainder of a Gauss formula $I_n(f)$ satisfies

$$\exists \xi \in [a, b] \text{ s.t. } E_n^G(f) = \frac{f^{(2n)}(\xi)}{(2n)!} \int_a^b \rho(x) v_n^2(x) dx, \quad (7.29)$$

where v_n is the node polynomial that defines I_n .

Proof. Not required. \square

7.5 Problems

7.5.1 Theoretical questions

I. Simpson's rule.

- (a) Show that on $[-1, 1]$ Simpson's rule can be obtained as follows

$$\int_{-1}^1 y(t) dt = \int_{-1}^1 p_3(y; -1, 0, 0, 1; t) dt + E^S(y),$$

where $y \in \mathcal{C}^4[-1, 1]$ and $p_3(y; -1, 0, 0, 1; t)$ is the interpolation polynomial of y with interpolation conditions $p_3(-1) = y(-1)$, $p_3(0) = y(0)$, $p_3'(0) = y'(0)$, and $p_3(1) = y(1)$.

- (b) Derive $E^S(y)$.
 (c) Using (a), (b) and a change of variable, derive the composite Simpson's rule and prove the theorem on its error estimation.

II. Estimate the number of subintervals required to approximate $\int_0^1 e^{-x^2} dx$ to 6 correct decimal places, i.e. the absolute error is no greater than 0.5×10^{-6} ,

- (a) by the composite trapezoidal rule,
 (b) by the composite Simpson's rule.

III. Gauss-Laguerre quadrature formula.

- (a) Construct a polynomial $\pi_2(t) = t^2 + at + b$ that is orthogonal to \mathbb{P}_1 with respect to the weight function $\rho(t) = e^{-t}$, i.e.

$$\forall p \in \mathbb{P}_1, \quad \int_0^{+\infty} p(t)\pi_2(t)\rho(t)dt = 0.$$

(*hint*: $\int_0^{+\infty} t^m e^{-t} dt = m!$)

- (b) Derive the two-point Gauss-Laguerre quadrature formula

$$\int_0^{+\infty} f(t)e^{-t}dt = w_1f(t_1) + w_2f(t_2) + E_2(f)$$

and express $E_2(f)$ in terms of $f^{(4)}(\tau)$ for some $\tau > 0$.

- (c) Apply the formula in (b) to approximate

$$I = \int_0^{+\infty} \frac{1}{1+t} e^{-t} dt.$$

Use the remainder to estimate the error and compare your estimate with the true error. With the true error, identify the unknown quantity τ contained in $E_2(f)$.

(*hint*: use the exact value $I = 0.596347361 \dots$)

Bibliography

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