Exercises

1. Show that the trapezoidal rule (4.4) is exact if the integrand $f(x)$ is a polynomial of degree no higher than first.

2.* Prove the result formulated in Remark 4.1.

   Hint. Show that any quadrature formula from the corresponding family can be represented as a linear combination of a number of trapezoidal formulae.

3. Show that for a nonuniform grid that satisfies $x_{k+1} - x_k \leq h = \text{const}$, the use of piecewise quadratic interpolation leads to a generalization of the Simpson formula that will only be third order accurate, i.e., will have $\mathscr{O}(M_3 h^3)$ error as $h \longrightarrow 0$, where $M_3 = \max |f'''(x)|$.

4. Construct an example of an infinitely smooth function $f(x)$, for which the error of the Simpson quadrature formula is still $\mathscr{O}(h^4)$.

4.2 Quadrature Formulae with No Saturation. Gaussian Quadratures

When we studied the interpolation of functions in Chapter 2, we first discovered that the conventional piecewise polynomial algebraic interpolation normally gets saturated by smoothness, i.e., exhibits only a fixed rate of convergence as the grid is refined irrespective of how smooth the interpolated function is. In its own turn, this property of interpolation gives rise to the saturation of the quadrature formulae by smoothness[1] that we described in Section 4.1. Later in Chapter 3, we introduced the trigonometric interpolation and showed that it does not get saturated by smoothness. In other words, it self-adjusts the accuracy of approximation to the regularity of the interpolated function, provided that the latter is periodic. In the non-periodic case, a direct analogue of the trigonometric interpolation is algebraic interpolation on Chebyshev nodes, e.g., on the Chebyshev-Gauss grid or on the Chebyshev-Gauss-Lobatto grid, see Section 3.2. Algebraic interpolation of this type does not get saturated by smoothness, and it is therefore natural to expect that if a quadrature formula is built based on the Chebyshev interpolation, then it will not be prone to saturation either. This expectation does, in fact, prove correct, and the corresponding family of quadrature formulae is commonly referred to as Gaussian quadratures. In this section, we introduce and study some examples of Gaussian quadratures. The material presented hereafter is based on the more advanced considerations of Chapter 3 and can be skipped during the first reading.

Chebyshev polynomials $T_k(x) \overset{\text{def}}{=} \cos(k \arccos x)$, $k = 0, 1, 2, \ldots$, were discussed in Section 3.2 in the context of interpolation. They are algebraic polynomials of degree k defined on the interval $-1 \leq x \leq 1$. An arbitrary interval $a \leq x \leq b$ can be mapped

[1] With the exception of the Newton-Cotes formulae applied to periodic functions.

onto $[-1,1]$ by a simple linear transformation: $x = \frac{a+2}{2} + t\frac{b-a}{2}$, where $-1 \le t \le 1$. Therefore, analyzing both interpolation and quadratures only on the interval $[-1,1]$ (as opposed to $[a,b]$) does not imply any loss of generality.

The $n+1$ roots of the Chebyshev polynomial $T_{n+1}(x)$ on the interval $[-1,1]$ are given by the formula:

$$x_m = \cos\frac{\pi(2m+1)}{2(n+1)}, \quad m = 0,1,2,\ldots,n, \tag{4.17}$$

and are referred to as the Chebyshev-Gauss nodes. The $n+1$ extrema of the Chebyshev polynomial $T_n(x)$ are given by the formula:

$$x_m = \cos\frac{\pi}{n}m, \quad m = 0,1,2,\ldots,n, \tag{4.18}$$

and are referred to as the Chebyshev-Gauss-Lobatto nodes. To employ Chebyshev polynomials in the context of numerical quadratures, we will additionally need their orthogonality property given by Lemma 4.1.

LEMMA 4.1
Chebyshev polynomials are orthogonal on the interval $-1 \le x \le 1$ with the weight $w(x) = 1/\sqrt{1-x^2}$, i.e., the following equalities hold for $k, l = 0,1,2,\ldots$:

$$\int_{-1}^{1} \frac{T_k(x)T_l(x)}{\sqrt{1-x^2}}dx = \begin{cases} \pi, & k = l = 0, \\ \pi/2, & k = l \ne 0, \\ 0, & k \ne l. \end{cases} \tag{4.19}$$

PROOF Let $x = \cos\varphi \;\Leftrightarrow\; \varphi = \arccos x$. Changing the variable in the integral, we obtain:

$$\int_{-1}^{1} \frac{T_k(x)T_l(x)}{\sqrt{1-x^2}}dx = \int_{\pi}^{0} \frac{\cos(k\varphi)\cos(l\varphi)}{|\sin\varphi|}(-\sin\varphi)d\varphi = \int_{0}^{\pi} \cos(k\varphi)\cos(l\varphi)d\varphi$$
$$= \frac{1}{2}\int_{0}^{\pi}[\cos(k+l)\varphi + \cos(k-l)\varphi]d\varphi = \begin{cases} \pi, & k = l = 0, \\ \pi/2, & k = l \ne 0, \\ 0, & k \ne l, \end{cases}$$

because Chebyshev polynomials are only considered for $k \ge 0$ and $l \ge 0$. ∎

Let the function $f = f(x)$ be defined for $-1 \le x \le 1$. We will approximate its definite integral over $[-1,1]$ taken with the weight $w(x) = 1/\sqrt{1-x^2}$ by integrating the Chebyshev interpolating polynomial $P_n(x,f)$ built on the Gauss nodes (4.17):

$$\int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}}dx \approx \int_{-1}^{1} \frac{P_n(x,f)}{\sqrt{1-x^2}}dx. \tag{4.20}$$

The key point, of course, is to obtain a convenient expression for the integral on the right-hand side of formula (4.20) via the function values $f(x_m)$, $m = 0,1,2,\ldots,m$, sampled on the Gauss grid (4.17). It is precisely the introduction of the weight $w(x) = 1/\sqrt{1-x^2}$ into the integral (4.20) that enables a particularly straightforward integration of the interpolating polynomial $P_n(x, f)$ over $[-1,1]$.

LEMMA 4.2
Let the function $f = f(x)$ be defined on $[-1,1]$, and let $P_n(x, f)$ be its algebraic interpolating polynomial on the Chebyshev-Gauss grid (4.17). Then,

$$\int_{-1}^{1} \frac{P_n(x,f)}{\sqrt{1-x^2}}dx = \frac{\pi}{n+1}\sum_{m=0}^{n} f(x_m). \tag{4.21}$$

PROOF Recall that $P_n(x, f)$ is an interpolating polynomial of degree no higher than n built for the function $f(x)$ on the Gauss grid (4.17). The grid has a total of $n+1$ nodes, and the polynomial is unique. As shown in Section 3.2.3, see formulae (3.62) and (3.63) on page 76, $P_n(x, f)$ can be represented as:

$$P_n(x,f) = \sum_{k=0}^{n} a_k T_k(x),$$

where $T_k(x)$ are Chebyshev polynomials of degree k, and the coefficients a_k are given by:

$$a_0 = \frac{1}{n+1}\sum_{m=0}^{n} f_m T_0(x_m) \quad \text{and} \quad a_k = \frac{2}{n+1}\sum_{m=0}^{n} f_m T_k(x_m), \ k = 1,\ldots,n.$$

Accordingly, it will be sufficient to show that equality (4.21) holds for all individual $T_k(x)$, $k = 0,1,2,\ldots,n$:

$$\int_{-1}^{1} \frac{T_k(x)}{\sqrt{1-x^2}}dx = \frac{\pi}{n+1}\sum_{m=0}^{n} T_k(x_m). \tag{4.22}$$

Let $k = 0$, then $T_0(x) \equiv 1$. In this case Lemma 4.1 implies that the left-hand side of (4.22) is equal to π, and the right-hand side also appears equal to π by direct substitution. For $k > 0$, orthogonality (4.19) means that the left-hand side of (4.22) is equal to zero. To prove that the right-hand side is zero as well, we employ formula (3.22). The range of summation in (3.22) is from $m = 0$ to $m = N-1$, where $N = 2(n+1)$. As, however, cosine is an even function, the same result will hold for half the summation range and any $k = 1,2,\ldots,2n+1$:

$$\begin{aligned}\sum_{m=0}^{n} T_k(x_m) &= \sum_{m=0}^{n} \cos\left(k \arccos\left[\cos\frac{\pi(2m+1)}{2(n+1)}\right]\right) \\ &= \sum_{m=0}^{n} \cos\left(k\frac{\pi(2m+1)}{2(n+1)}\right) = \sum_{m=0}^{n} \cos\left(k\frac{2\pi m}{2(n+1)} + k\frac{\pi}{2(n+1)}\right) = 0.\end{aligned}$$

This implies, in particular, that the right-hand side of (4.22) is zero for all $k = 1, 2, \dots, n$. Thus, we have established equality (4.21). ∎

Lemma 4.21 allows us to recast the approximate expression (4.20) for the integral $\int_{-1}^{1} f(x)w(x)dx$ as follows:

$$\int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}} dx \approx \frac{\pi}{n+1} \sum_{m=0}^{n} f(x_m). \tag{4.23}$$

Formula (4.23) is known as the Gaussian quadrature formula with the weight $w(x) = 1/\sqrt{1-x^2}$ on the Chebyshev-Gauss grid (4.17). It has a particularly simple structure, which is very convenient for implementation. In practice, if we need to evaluate the integral $\int_{-1}^{1} f(x)dx$ for a given $f(x)$ with no weight, we introduce a new function $g(x) = f(x)\sqrt{1-x^2}$ and then rewrite formula (4.23) as:

$$\int_{-1}^{1} f(x)dx = \int_{-1}^{1} \frac{g(x)}{\sqrt{1-x^2}} dx \approx \frac{\pi}{n+1} \sum_{m=0}^{n} g(x_m).$$

A key advantage of the Gaussian quadrature (4.23) compared to the quadrature formulae studied previously in Section 4.1 is that the Gaussian quadrature does not get saturated by smoothness. Indeed, according to the following theorem (see also Remark 4.2 right after the proof of Theorem 4.5), the integration error automatically adjusts to the regularity of the integrand.

THEOREM 4.5

Let the function $f = f(x)$ be defined for $-1 \le x \le 1$; let it have continuous derivatives up to the order $r > 0$, and a square integrable derivative of order $r+1$:

$$\int_{-1}^{1} \left[f^{(r+1)}(x) \right]^2 dx < \infty.$$

Then, the error of the Gaussian quadrature (4.23) can be estimated as:

$$\left| \int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}} dx - \frac{\pi}{n+1} \sum_{m=0}^{n} f(x_m) \right| \le \pi \frac{\zeta_n}{n^{r-1/2}}, \tag{4.24}$$

where $\zeta_n = o(1)$ as $n \longrightarrow \infty$.

PROOF The proof of inequality (4.24) is based on the error estimate (3.65) obtained in Section 3.2.4 (see page 77) for the Chebyshev algebraic interpolation. Namely, let $R_n(x) = f(x) - P_n(x, f)$. Then, under the assumptions of the current theorem we have:

$$\max_{-1\le x\le 1}|R_n(x)| \le \frac{\zeta_n}{n^{r-1/2}}, \quad \text{where} \quad \zeta_n = o(1), \quad n \longrightarrow \infty. \tag{4.25}$$

Consequently,

$$\begin{aligned}\left|\int_{-1}^{1}\frac{f(x)}{\sqrt{1-x^2}}dx - \frac{\pi}{n+1}\sum_{m=0}^{n} f(x_m)\right| &= \left|\int_{-1}^{1}\frac{f(x)}{\sqrt{1-x^2}}dx - \int_{-1}^{1}\frac{P_n(x,f)(x)}{\sqrt{1-x^2}}dx\right| \\ &\le \int_{-1}^{1}\frac{|f(x)-P_n(x,f)|}{\sqrt{1-x^2}}dx \le \max_{-1\le x\le 1}|R_n(x)|\cdot\int_{-1}^{1}\frac{dx}{\sqrt{1-x^2}} = \pi\frac{\zeta_n}{n^{r-1/2}},\end{aligned}$$

which yields the desired estimate (4.24). ∎

Theorem 4.5 implies, in particular, that if the function $f = f(x)$ is infinitely differentiable on $[-1,1]$, then the Gaussian quadrature (4.23) exhibits a spectral rate of convergence as the dimension of the grid n increases. In other words, the integration error in (4.24) will decay faster than $\mathscr{O}(n^{-r})$ for any $r > 0$ as $n \longrightarrow \infty$.

REMARK 4.2 Error estimate (4.25) for the algebraic interpolation on Chebyshev grids can, in fact, be improved. According to formula (3.67), see Remark 3.2 on page 78, instead of inequality (4.25) we can write:

$$\max_{-1\le x\le 1}|R_n(x)| = o\left(\frac{\ln n}{n^{r+1/2}}\right) \quad \text{as} \quad n \longrightarrow \infty.$$

Then, the same argument as employed in the proof of Theorem 4.5 yields an improved convergence result for Gaussian quadratures:

$$\left|\int_{-1}^{1}\frac{f(x)}{\sqrt{1-x^2}}dx - \frac{\pi}{n+1}\sum_{m=0}^{n} f(x_m)\right| = o\left(\frac{\pi\ln n}{n^{r+1/2}}\right) \quad \text{as} \quad n \longrightarrow \infty,$$

where $r+1$ is the maximum number of derivatives that the integrand $f(x)$ has on the interval $-1 \le x \le 1$. However, even this is not the best estimate yet.

As shown in Section 3.2.7, by combining the Jackson inequality [Theorem 3.8, formula (3.79)], the Lebesgue inequality [Theorem 3.10, formula (3.80)], and estimate (3.83) for the Lebesgue constants given by the Bernstein theorem [Theorem 3.12], one can obtain the following error estimate for the Chebyshev algebraic interpolation:

$$\max_{-1\le x\le 1}|R_n(x)| = \mathscr{O}\left(\frac{\ln(n+1)}{n^{r+1}}\right), \quad \text{as} \quad n \longrightarrow \infty,$$

provided only that the derivative $f^{(r)}(x)$ of the function $f(x)$ is Lipshitz-continuous. Consequently, for the error of the Gaussian quadrature we have:

$$\left| \int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}} dx - \frac{\pi}{n+1} \sum_{m=0}^{n} f(x_m) \right| = \mathscr{O}\left(\pi \frac{\ln(n+1)}{n^{r+1}} \right), \quad \text{as} \quad n \longrightarrow \infty. \tag{4.26}$$

Estimate (4.26) implies, in particular, that the Gaussian quadrature (4.23) converges at least for any Lipshitz-continuous function (page 87), and that the rate of decay of the error is not slower than $\mathscr{O}(n^{-1}\ln(n+1))$ as $n \longrightarrow \infty$. Otherwise, for smoother functions the convergence speeds up as the regularity increases, and becomes spectral for infinitely differentiable functions. ▯

REMARK 4.3 When proving Lemma 4.2, we have, in fact, shown that equality (4.22) holds for all Chebyshev polynomials $T_k(x)$ up to the degree $k = 2n+1$ and not only up to the degree $k = n$. This circumstance reflects on another important property of the Gaussian quadrature (4.23). It happens to be exact, i.e., it generates no error, for any algebraic polynomial of degree no higher than $2n+1$ on the interval $-1 \leq x \leq 1$. In other words, if $Q_{2n+1}(x)$ is a polynomial of degree $\leq 2n+1$, then

$$\int_{-1}^{1} \frac{Q_{2n+1}(x)}{\sqrt{1-x^2}} dx = \frac{\pi}{n+1} \sum_{m=0}^{n} Q_{2n+1}(x_m).$$

Moreover, it is possible to show that the Gaussian quadrature (4.23) is optimal in the following sense. Consider a family of the quadrature formulae on $[-1,1]$:

$$\int_{-1}^{1} f(x)w(x)dx \approx \sum_{j=0}^{n} \alpha_j f(x_j), \tag{4.27}$$

where the dimension n is fixed, the weight $w(x)$ is defined as before, $w(x) = 1/\sqrt{1-x^2}$, and both the nodes x_j and the coefficients α_j, $j = 0,1,\dots,n$ are to be determined. Require that this quadrature be exact for the polynomials of the highest degree possible. Then, it turns out that the corresponding degree will be equal to $2n+1$, while the nodes x_j will coincide with those of the Chebyshev-Gauss grid (4.17), and the coefficients α_j will all be equal to $\pi/(n+1)$. Altogether, quadrature (4.27) will coincide with (4.23). ▯

Exercises

1. Prove an analogue of Lemma 4.2 for the Gaussian quadrature on the Chebyshev-Gauss-Lobatto grid (4.18). Namely, let $\tilde{P}_n(x,f) = \sum_{k=0}^{n} \tilde{a}_k T_k(x)$ be the corresponding interpolating polynomial (constructed in Section 3.2.6). Show that

$$\int_{-1}^{1} \frac{\tilde{P}_n(x,f)}{\sqrt{1-x^2}} dx = \frac{\pi}{n} \sum_{m=0}^{n} \beta_m f(x_m),$$

where $\beta_0 = \beta_n = 1/2$ and $\beta_m = 1$ for $m = 1, 2, \ldots, m-1$.

4.3 Improper Integrals. Combination of Numerical and Analytical Methods

Even for the simplest improper integrals, a direct application of the quadrature formulae may encounter serious difficulties. For example, the trapezoidal rule (4.4):

$$\int_a^b f(x)dx \approx \frac{b-a}{n}\left(\frac{f_0}{2} + f_1 + \ldots + f_{n-1} + \frac{f_n}{2}\right)$$

will fail for the case $a = 0, b = 1$, and $f(x) = \cos x/\sqrt{x}$, because $f(x)$ has a singularity at $x = 0$ and consequently, $f_0 = f(0)$ is not defined. Likewise, the Simpson formula (4.13) will fail. For the Gaussian quadrature (4.23), the situation may seem a little better at a first glance, because the Chebyshev-Gauss nodes (4.17) do not include the endpoints of the interval. However, the unboundedness of the function and its derivatives will still prevent one from obtaining any reasonable error estimates. At the same time, the integral itself: $\int_0^1 \frac{\cos x}{\sqrt{x}} dx$, obviously exists, and procedures for its efficient numerical approximation need to be developed.

To address the difficulties that arise when computing the values of improper integrals, it is natural to try and employ a combination of analytical and numerical techniques. The role of the analytical part is to reduce the original problem to a new problem that would only require one to evaluate the integral of a smooth and bounded function. The latter can then be done on a computer with the help of a quadrature formula. In the previous example, we can first use the integration by parts:

$$\int_0^1 \frac{\cos x}{\sqrt{x}} dx = \cos x(2\sqrt{x})\Big|_0^1 + \int_0^1 s\sqrt{x}\sin x dx,$$

and subsequently approximate the integral on the right-hand side to a desired accuracy using any of the quadrature formulae introduced in Section 4.1 or 4.2.

An alternative approach is based on splitting the original integral into two:

$$\int_0^1 \frac{\cos x}{\sqrt{x}} dx = \int_0^c \frac{\cos x}{\sqrt{x}} dx + \int_c^1 \frac{\cos x}{\sqrt{x}} dx, \tag{4.28}$$

where $c > 0$ can be considered arbitrary as of yet. To evaluate the first integral on the right-hand side of equality (4.28), we can use the Taylor expansion:

$$\cos x = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \ldots.$$