Gaussian Quadrature and the Eigenvalue Problem

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1. Introduction

Numerical integration or quadrature is the approximation of an integral $\int f\,d\mu$ by another integral $\int \hat{f}\,d\mu$, where $\hat{f}$ is a function that is "close" to f and whose integral is known.[1] It frequently happens that $\int \hat{f}\,d\mu$ can be expressed in the form

$$\sum_{k=1}^{n} w_k f(x_k),$$

where the **nodes** x_k belong to the range of integration and the **weights** w_k are computable. For example, this kind of formula always results when $\hat{f}$ is a polynomial of degree less than n that **interpolates** to f at the nodes; i.e., $\hat{f}(x_k) = f(x_k)$ for $k = 1,\ldots,n$.

As we show below, once the nodes x_k are fixed, it is easy to choose the weights w_k so that if f is any polynomial of degree less than n, then

$$\int f\,d\mu = \sum_{k=1}^{n} w_k f(x_k).$$

However, if the nodes are carefully chosen (*Gaussian* quadrature), then this formula holds with equality for all polynomials f of degree less than $2n$. To explain how to do this leads us into the theory of orthogonal polynomials. The key results are Theorems 6 and 7. They are illustrated in the context of the Chebyshev polynomials in Example 11, where the nodes and weights for Chebyshev–Gauss quadrature are obtained. The remainder of the paper is devoted to showing that for Gaussian quadrature, the kth node x_k is the kth eigenvalue of a tridiagonal matrix J_n, and the kth weight w_k is simply related to the first component of the corresponding ortho*normal* eigenvector. Simple MATLAB functions are given that compute the nodes and weights for Hermite–Gauss, Laguerre–Gauss, and Legendre–Gauss quadrature.

2. Polynomial Interpolation

Given distinct real numbers $x_1,\ldots,x_n$, the **Lagrange fundamental interpolating polynomials** are

$$\ell_k(x) := \frac{(x-x_1)\cdots(x-x_{k-1})(x-x_{k+1})\cdots(x-x_n)}{(x_k-x_1)\cdots(x_k-x_{k-1})(x_k-x_{k+1})\cdots(x_k-x_n)}.$$

[1]Readers unfamiliar with measure theory can replace $\int f(x)\,d\mu(x)$ with $\int f(x)w(x)\,dx$, where the **weight function** $w(x)$ is positive for all but at most finitely many values of x in the interval of interest. Typical examples include

$$\begin{array}{lllll} w(x) = e^{-x^2}, & -\infty < x < \infty, & \quad & w(x) = 1/\sqrt{1-x^2}, & -1 < x < 1, \\ w(x) = e^{-x}, & 0 \le x < \infty, & & w(x) = 1, & -1 \le x \le 1, \end{array}$$

where it is understood that $w(x) = 0$ for values of x outside the indicated range of interest. In addition, if B is a subset of $\mathbb{R}$, then $\mu(B) := \int_B w(x)\,dx$. In particular, $\mu(\mathbb{R}) = \int_{-\infty}^{\infty} w(x)\,dx$.

Then ℓ_k is a polynomial of degree $n-1$ that also satisfies

$$\ell_k(x_i) = \delta_{ki} := \begin{cases} 1, & i = k, \\ 0, & i \ne k, \end{cases}$$

where δ is the **Kronecker delta**. Using these polynomials, if we are given a real or complex-valued function f defined on $\mathbb{R}$, then

$$\hat{f}(x) := \sum_{k=1}^{n} f(x_k)\ell_k(x), \tag{1}$$

is a polynomial of degree less than n that interpolates to f at the points $x_1,\ldots,x_n$; i.e., $\hat{f}(x_k) = f(x_k)$ for $k = 1,\ldots,n$.

Proposition 1. *The interpolating polynomial $\hat{f}$ is unique.*

Proof. Let g be another interpolating polynomial of degree less than n. Then $h := \hat{f} - g$ is a polynomial of degree less than n but has n roots since

$$h(x_k) = \hat{f}(x_k) - g(x_k) = f(x_k) - f(x_k) = 0, \quad k = 1,\ldots,n.$$

Therefore, $h = 0$; i.e., $\hat{f} = g$. □

Remark. As a consequence of the proposition, if f is a *polynomial* with $\deg f \le n-1$, then $\hat{f} = f$.

3. Interpolatory Quadrature

Let μ be a measure on $\mathbb{R}$ such that $\int |x|^k\,d\mu(x) < \infty$ for $k = 0,1,2,\ldots.$ This guarantees that for any polynomial p, $\int p\,d\mu$ exits. To avoid the uninteresting situations, we assume that for any finite set G, $\mu(\mathbb{R}\setminus G) > 0$. When $G = \varnothing$, this implies $\mu(\mathbb{R}) > 0$.

Given a function f and its interpolating polynomial $\hat{f}$ of degree less than n, we can write

$$\begin{aligned} \int \hat{f}(x)\,d\mu(x) &= \int \left[\sum_{k=1}^{n} f(x_k)\ell_k(x)\right] d\mu(x), \quad \text{by (1)}, \\ &= \sum_{k=1}^{n} f(x_k)\int \ell_k(x)\,d\mu(x). \end{aligned}$$

If we define the weights

$$w_k := \int \ell_k\,d\mu, \quad k = 1,\ldots,n, \tag{2}$$

then

$$\int \hat{f}\,d\mu = \sum_{k=1}^{n} w_k f(x_k). \tag{3}$$

Lemma 2. *If f is a polynomial of degree less than n, then*

$$\int f\,d\mu = \sum_{k=1}^{n} w_k f(x_k). \tag{4}$$

Proof. By the Remark following Proposition 1, since f is a polynomial of degree less than n, $f = \hat{f}$. Hence $\int f\,d\mu = \int \hat{f}\,d\mu$, which is given by (3). □

Example 3 (Newton–Cotes). When the nodes x_k are equally spaced in a finite interval of integration, we obtain a **Newton–Cotes formula**. The case $n = 3$ corresponds to **Simpson's rule**. To derive it, we first work out the special case with nodes spaced one unit apart and symmetrically placed around $x = 0$; i.e., $x_1 = -1$, $x_2 = 0$, and $x_3 = 1$. Then

$$\begin{aligned}
\ell_1(x) &= \frac{(x-x_2)(x-x_3)}{(x_1-x_2)(x_1-x_3)} = \frac{(x-0)(x-1)}{((-1)-0)((-1)-1)} \\
&= \tfrac{1}{2}x(x-1) \\
\ell_2(x) &= \frac{(x-x_1)(x-x_3)}{(x_2-x_1)(x_2-x_3)} = \frac{(x-(-1))(x-1)}{(0-(-1))(0-1)} \\
&= 1-x^2 \\
\ell_3(x) &= \frac{(x-x_1)(x-x_2)}{(x_3-x_1)(x_3-x_2)} = \frac{(x-(-1))(x-0)}{(1-(-1))(1-0)} \\
&= \tfrac{1}{2}x(x+1).
\end{aligned}$$

Next, since x is an odd function and x^2 is an even function,

$$w_1 = \int_{-1}^{1} \ell_1(x)\,dx = \tfrac{1}{2}\int_{-1}^{1} x^2\,dx = \int_0^1 x^2\,dx = 1/3.$$

Similarly,

$$w_2 = \int_{-1}^{1} \ell_2(x)\,dx = 2\int_0^1 1-x^2\,dx = 4/3.$$

Since $\ell_3(x) = \ell_1(-x)$,

$$w_3 = \int_{-1}^{1} \ell_1(-x)\,dx = \int_{-1}^{1} \ell_1(x)\,dx = w_1 = 1/3.$$

So, for any polynomial p with $\deg p \le 2$,

$$\int_{-1}^{1} p(x)\,dx = [p(-1)+4p(0)+p(1)]/3.$$

Notice that since x^3 is odd, the above formula actually holds for all polynomials of degree less than or equal to 3. To integrate $p(t)$ over an arbitrary interval $[a,b]$, use the change of variable $t = a+(b-a)(x+1)/2$; $dt = [(b-a)/2]\,dx$, to write

$$\int_a^b p(t)\,dt = \frac{b-a}{2}\int_{-1}^{1}\widetilde{p}(x)\,dx = \frac{b-a}{6}\Big[\widetilde{p}(-1)+4\widetilde{p}(0)+\widetilde{p}(1)\Big],$$

where

$$\widetilde{p}(x) := p\Big(a+\frac{b-a}{2}(x+1)\Big).$$

It follows that

$$\int_a^b p(t)\,dt = \frac{b-a}{6}\Big[p(a)+4p\Big(\frac{a+b}{2}\Big)+p(b)\Big].$$

Using the same ideas with $n = 5$, you can derive **Boole's rule**: For polynomials p with $\deg p \le 5$,

$$\begin{aligned}
&\int_a^b p(t)\,dt \\
&\quad = \frac{b-a}{90}\big[7f(x_1)+32f(x_2)+12f(x_3)+32f(x_4)+7f(x_5)\big],
\end{aligned}$$

where $x_k = a+(k-1)h$ for $k = 1,\dots,5$ and $h = (b-a)/(n-1)$.

Lemma 4. *For the polynomial of degree n*

$$\zeta(x) := (x-x_1)\cdots(x-x_n),$$

we have $\int \zeta^2\,d\mu > 0$.

Proof. Suppose otherwise that $\int \zeta^2\,d\mu = 0$. Then since $\zeta^2 \ge 0$, $\zeta^2 = 0$ μ-a.e.; i.e., if $G := \{x : \zeta(x)^2 = 0\}$, then $\mu(\mathbb{R}\setminus G) = 0$. But $G = \{x_1,\dots,x_n\}$ is a finite set, and we have assumed $\mu(\mathbb{R}\setminus G) > 0$ for finite sets G. □

Lemma 5. *If* (4) *holds for all polynomials of degree less than* $2n$*, then the weights w_i must be positive.*

Proof. First, from the Kronecker delta property of $\ell_i(x_k)$,

$$w_i := \sum_{k=1}^{n} w_k \ell_i(x_k)^2.$$

Second, since we are assuming (4) holds for polynomials of degree less than $2n$, and since $\deg \ell_i^2 = 2n-2$, we can write

$$\sum_{k=1}^{n} w_k \ell_i(x_k)^2 = \int \ell_i^2\,d\mu > 0$$

by the argument used in the proof of Lemma 4. □

Suppose we take $f = \zeta^2$ in (4). Then by Lemma 4 the left-hand side is positive, while the right-hand size is zero, since $\zeta(x_k) = 0$ for $k = 1,\dots,n$. Since $\deg \zeta^2 = 2n$, we have shown that (4) cannot hold for all polynomials of degree greater than or equal to $2n$.

Suppose that (4) holds for all polynomials of degree less than $2n$. Then in particular it must hold for $f = q\zeta$ whenever q is a polynomial with $\deg q < n$. In this case, (4) reduces to

$$\int q\zeta\,d\mu = 0, \tag{5}$$

since $\zeta(x_k) = 0$ for $k = 1,\dots,n$.

For any polynomial f, we can always divide it by ζ in the sense that there exist polynomials q and r such that

$$f = q\zeta + r, \quad \deg r < \deg \zeta = n. \tag{6}$$

Note that since $\deg r \le n-1$, Lemma 2 implies

$$\int r\,d\mu = \sum_{k=1}^{n} w_k r(x_k).$$

Furthermore,

$$\begin{aligned} r(x_k) &= f(x_k) - q(x_k)\zeta(x_k) \\ &= f(x_k), \end{aligned}$$

since $\zeta(x_k) = 0$. Hence,

$$\int r\,d\mu = \sum_{k=1}^{n} w_k f(x_k).$$

We can now write

$$\begin{aligned} \int f\,d\mu &= \int (q\zeta + r)\,d\mu \\ &= \int q\zeta\,d\mu + \int r\,d\mu \\ &= \int q\zeta\,d\mu + \sum_{k=1}^{n} w_k f(x_k). \end{aligned}$$

This reduces to (4) if the integral on the right is zero; i.e., if (5) holds. Now, if $\deg f < 2n$, then q in (6) must satisfy $\deg q < n$. Hence, if (5) holds for all such q, then (4) holds for f. We thus have the following result.

Theorem 6. *Equation* (4) *holds for all polynomials f with $\deg f < 2n$ if and only if* (5) *holds for all polynomials q with $\deg q < n$. Furthermore,* (4) *cannot hold for all polynomials of degree greater than or equal to $2n$.*

4. Orthogonal Polynomials

Examination of (5) suggests that for polynomials p and q, we define their **inner product**[2]

$$\langle p, q\rangle := \int pq\,d\mu.$$

For use below, the **norm** of p is $\|p\| := \langle p, p\rangle^{1/2}$. With our inner-product notation, (5) says that ζ is orthogonal to the subspace

$$\mathbb{P}_{n-1} := \operatorname{span}\{1, x, \ldots, x^{n-1}\}$$

of polynomials of degree less than n.

Let us apply the Gram–Schmidt procedure to construct polynomials

$$\varphi_n(x) := x^n - \sum_{k=0}^{n-1} \frac{\langle x^n, \varphi_k\rangle}{\langle \varphi_k, \varphi_k\rangle}\varphi_k(x), \quad n \geq 1, \tag{7}$$

where $\varphi_0(x) := 1$. It is easy to check that φ_n is orthogonal to φ_i for $i = 0, \ldots, n-1$. Furthermore, it is easy to see by induction that

$$\operatorname{span}\{\varphi_0, \ldots, \varphi_k\} = \operatorname{span}\{1, x, \ldots, x^k\} = \mathbb{P}_k, \quad k = 0, 1, \ldots.$$

In particular, it follows that φ_n is orthogonal to $\mathbb{P}_{n-1}$ for $n \geq 1$.

[2] We are considering real-valued functions here. In the complex case,

$$\langle p, q\rangle := \int p\,\bar{q}\;d\mu,$$

where the overbar denotes complex conjugation.

Theorem 7. *For $n \geq 1$, the polynomial φ_n has n distinct real roots.*

Proof. Since φ_n and 1 are orthogonal by construction, $\int \varphi_n\,d\mu = 0$. We first show that φ_n has at least one real root. Suppose not. Then φ_n is either always positive or always negative as a consequence of the intermediate value theorem. However, the condition that φ_n be of one sign along with the condition $\int \varphi_n\,d\mu = 0$ implies $\varphi_n(x) = 0$ for μ-a.e. x, contradicting the earlier assumption that $\mu(\mathbb{R}) > 0$. Thus, φ_n has at least one real root. Let $x_1, \ldots, x_k$ be real roots of φ_n, where $k < n$. If we put

$$p(x) := (x - x_1)\cdots(x - x_k),$$

then p is a polynomial of degree less than n, and must therefore be orthogonal to φ_n. However, since the x_i are roots of φ_n, we can write $\varphi_n(x) = p(x)q(x)$ for some polynomial q with $\deg q \geq 1$. Now write

$$0 = \int \varphi_n p\,d\mu = \int qp^2\,d\mu.$$

If q has no real roots, it is of one sign, and so qp^2 is either always nonnegative or always nonpositive. Furthermore, since the above integral is zero, we must then have $qp^2 = 0$ μ-a.e.; i.e., if $G := \{qp^2 = 0\}$, then $\mu(\mathbb{R}\setminus G) = 0$. But this contradicts the earlier assumption that for finite sets G, $\mu(\mathbb{R}\setminus G) > 0$. We therefore conclude that φ_n cannot have fewer than n real roots.

It remains to show that the roots must be distinct. Suppose otherwise that some real root is repeated, say $x_n = x_{n-1}$. Then

$$\varphi_n(x) = (x - x_1)\cdots(x - x_{n-2})(x - x_{n-1})^2.$$

If we now redefine $p(x) := (x - x_1)\cdots(x - x_{n-2})$, then $\varphi_n(x) = p(x)(x - x_{n-1})^2$. Hence,

$$\begin{aligned} 0 &< \int p(x)^2(x - x_{n-2})^2\,d\mu(x) \\ &= \int \big[p(x)(x - x_{n-2})^2\big]\,p(x)\,d\mu(x) \\ &= \int \varphi_n(x)p(x)\,d\mu(x) \\ &= 0, \end{aligned}$$

where the last step follows because φ_n is orthogonal to all polynomials of degree less than n and $\deg p < n$. ☐

If we denote the roots of φ_n by $x_1, \ldots, x_n$, then φ_n is the ζ we seek for (5) to hold.

Proposition 8 (Discrete-Orthogonality). *For $0 \leq i, j < n$,*

$$\sum_{k=1}^{n} w_k \varphi_i(x_k)\varphi_j(x_k) = \langle \varphi_i, \varphi_j\rangle = \|\varphi_i\|\,\|\varphi_j\|\delta_{ij}, \tag{8}$$

where $x_1, \ldots, x_n$ are the distinct real roots of φ_n.

Proof. The equality on the right is obvious since φ_i and φ_j are orthogonal for $i \neq j$. To establish the equality on the left, write

$$\langle \varphi_i, \varphi_j\rangle = \int \varphi_i\varphi_j\,d\mu = \sum_{k=1}^{n} w_k \varphi_i(x_k)\varphi_j(x_k),$$

where the last equation follows because $\deg \varphi_i\varphi_j < 2n$. ☐

Corollary 9 (Dual Orthogonality). *The weights* $w_i := \int \ell_i \, d\mu$ *satisfy*

$$\sum_{k=0}^{n-1} \frac{\varphi_k(x_i)\varphi_k(x_j)}{\|\varphi_k\|^2} = \delta_{ij}/\sqrt{w_i w_j}, \quad 1 \le i, j \le n. \tag{9}$$

Proof. (Gautschi [2, p. 4].) Divide both sides of (8) by $\|\varphi_i\|\,\|\varphi_j\|$. The resulting equation can be expressed as the $n \times n$ matrix equation $Q'Q = I$, where $Q_{kj} := \sqrt{w_k}\varphi_j(x_k)/\|\varphi_j\|$. Since $QQ' = I$ as well, we can write

$$\delta_{kl} = (QQ')_{kl} = \sqrt{w_k w_l} \sum_{j=1}^{n-1} \frac{\varphi_j(x_k)\varphi_j(x_l)}{\|\varphi_j\|^2}.$$

Now change k to i, j to k, and l to j. □

Theorem 10 (Three-Term Recurrence Relation). *Suppose that* $\varphi_0, \varphi_1, \ldots$ *are orthogonal polynomials with* $\deg \varphi_n = n$ *and leading coefficient one. For* $n \ge 1$ *we have the three-term recurrence*

$$\varphi_{n+1}(x) = (x - a_n)\varphi_n(x) - b_n \varphi_{n-1}(x),$$

where

$$a_n := \frac{\langle x\varphi_n, \varphi_n \rangle}{\langle \varphi_n, \varphi_n \rangle} \text{ and } b_n := \frac{\langle \varphi_n, x\varphi_{n-1} \rangle}{\langle \varphi_{n-1}, \varphi_{n-1} \rangle} = \frac{\langle \varphi_n, \varphi_n \rangle}{\langle \varphi_{n-1}, \varphi_{n-1} \rangle} > 0.$$

We also have

$$\varphi_1(x) = (x - a_0)\varphi_0(x) = x - a_0,$$

where $a_0 := \langle x\varphi_0, \varphi_0 \rangle / \langle \varphi_0, \varphi_0 \rangle = \int x \, d\mu / \mu(\mathbb{R})$.

Proof. First note that the difference polynomial

$$\begin{aligned} D(x) &:= \varphi_{n+1}(x) - x\varphi_n(x) \\ &= \big(x^{n+1} + \cdots\big) - x\big(x^n + \cdots\big) \end{aligned}$$

is a polynomial of degree at most n. Hence, D can be expanded in terms of the orthogonal $\varphi_0, \ldots, \varphi_n$ as

$$\begin{aligned} D &= \sum_{k=0}^{n} \frac{\langle D, \varphi_k \rangle}{\langle \varphi_k, \varphi_k \rangle} \varphi_k \\ &= \sum_{k=0}^{n} \frac{\langle \varphi_{n+1} - x\varphi_n, \varphi_k \rangle}{\langle \varphi_k, \varphi_k \rangle} \varphi_k \\ &= -\sum_{k=0}^{n} \frac{\langle x\varphi_n, \varphi_k \rangle}{\langle \varphi_k, \varphi_k \rangle} \varphi_k, \quad \text{by orthogonality,} \\ &= -\sum_{k=0}^{n} \frac{\langle \varphi_n, x\varphi_k \rangle}{\langle \varphi_k, \varphi_k \rangle} \varphi_k \\ &= -\sum_{k=n-1}^{n} \frac{\langle \varphi_n, x\varphi_k \rangle}{\langle \varphi_k, \varphi_k \rangle} \varphi_k, \quad \text{by orthogonality,} \end{aligned}$$

since $\deg x\varphi_k(x) < n$ for $k < n-1$. Solving for φ_{n+1} yields the result using the definitions of a_n and b_n. The remaining formula for b_n results by observing that

$$\langle \varphi_n, x\varphi_{n-1} \rangle - \langle \varphi_n, \varphi_n \rangle = \langle \varphi_n, x\varphi_{n-1} - \varphi_n \rangle = 0$$

since $x\varphi_{n-1} - \varphi_n$ is of degree at most $n-1$ and therefore orthogonal to φ_n. □

Example 11. The **Chebyshev polynomials** $T_n(x)$ are defined as follows. For $-1 \le x \le 1$, put

$$T_n(x) := \cos(n \cos^{-1}(x)).$$

It is easy to see that $T_0(x) = 1$ and $T_1(x) = x$. We now show that the T_n satisfy the three-term recurrence

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x). \tag{10}$$

Put $\theta := \cos^{-1}(x)$ so that for $n \ge 1$, we can write

$$\begin{aligned} T_{n\pm1}(x) &= \cos([n \pm 1]\theta) \\ &= \cos(n\theta)\cos\theta \mp \sin(n\theta)\sin\theta \\ &= T_n(x) \cdot x \mp \sin(n\theta)\sin\theta. \end{aligned}$$

Hence,

$$T_{n+1}(x) + T_{n-1}(x) = 2xT_n(x),$$

and (10) follows. Although we originally defined $T_n(x)$ only for $-1 \le x \le 1$, if we start with $T_0(x) = 1$ and $T_1(x) = x$ and define $T_{n+1}(x)$ by (10) for $n \ge 1$, then $T_n(x)$ is a polynomial of degree n that is defined for all x.

We next show that T_n has n distinct real roots in $(-1, 1)$ that can be found by inspection. Recall that $\cos(\theta) = 0$ when θ is an odd multiple of $\pi/2$. Put

$$x_k := \cos\Big(\frac{2k-1}{2n}\pi\Big), \quad k = 1, \ldots, n,$$

so that $n\cos^{-1}(x_k) = (2k-1)\pi/2$. Then

$$T_n(x_k) = \cos(n\cos^{-1}(x_k)) = \cos\Big((2k-1)\frac{\pi}{2}\Big) = 0.$$

Our next task is to show that the T_n are orthogonal if $d\mu(x) = dx/\sqrt{1-x^2}$. In the integral

$$\langle T_n, T_m \rangle = \int_{-1}^{1} \frac{T_n(x)T_m(x)}{\sqrt{1-x^2}} \, dx,$$

make the change of variable $x = \cos\theta$, $dx = -\sin\theta \, d\theta$. Then

$$\begin{aligned} \langle T_n, T_m \rangle &= \int_{\pi}^{0} \frac{\cos(n\theta)\cos(m\theta)}{\sqrt{1-\cos^2\theta}} (-\sin\theta) \, d\theta \\ &= \int_{0}^{\pi} \cos(n\theta)\cos(m\theta) \, d\theta. \end{aligned}$$

Using the identity

$$\cos A \cos B = \tfrac{1}{2}[\cos(A-B) + \cos(A+B)],$$

it is easy to show that the above integral is zero for $n \ne m$.

Although the T_n are orthogonal, they do not have leading coefficient one as do the $\varphi_n(x)$. By writing out (10) for a few values of n, it is easy to see that the leading coefficient of T_n is 2^{n-1} for $n \ge 1$. Hence, $\varphi_n(x) = T_n(x)/2^{n-1}$. Dividing (10) by 2^n, we find that

$$\varphi_{n+1}(x) = x\varphi_n(x) - (1/4)\varphi_{n-1}(x), \quad n \ge 2.$$

Since $\varphi_1 = T_1$ and $\varphi_0 = T_0$, we also have

$$\varphi_2(x) = x\varphi_1(x) - (1/2)\varphi_0(x).$$

Hence, $a_n = 0$ for $n \geq 1$, while $b_1 = 1/2$ and $b_n = 1/4$ for $n \geq 2$.

We now show that the weights are all the same and equal to π/n. First, it is easy to see that for $n \geq 1$, $\|T_n\|^2 = \pi/2$, and hence, $\|\varphi_n\|^2 = \pi/2^{2n-1}$. The formula for w_i then follows from (9) with $j = i$ and some simplification.

We conclude this example by pointing out that the Chebyshev–Gauss nodes x_k can be generated as a vector (from largest to smallest) with the single MATLAB command `x=cos([1:2:2*n]*pi/(2*n))`.

In general, the nodes and weights cannot be found by inspection. It would seem that unless the φ_n have a special structure, in order to find the nodes x_i and weights w_i, we have to find the n distinct roots of φ_n to get the x_i and then compute the w_i using either the integral definition $w_i = \int \ell_i \, d\mu$ or (9). However, there is another way.

Theorem 12. *The w_i and x_i can be obtained from the* ***eigenvalue decomposition*** *of the symmetric, tridiagonal* ***Jacobi matrix***

$$J_n := \begin{bmatrix} a_0 & \sqrt{b_1} & & & \\ \sqrt{b_1} & a_1 & \sqrt{b_2} & & \\ & \sqrt{b_2} & \ddots & \ddots & \\ & & \ddots & a_{n-2} & \sqrt{b_{n-1}} \\ & & & \sqrt{b_{n-1}} & a_{n-1} \end{bmatrix},$$

where the a_n and b_n are as in the three-term recurrence Theorem 10. If $V'J_nV = \Lambda = \operatorname{diag}(\lambda_1, \ldots, \lambda_n)$, where $V'V = I$ is the $n \times n$ identity matrix, then $x_i = \lambda_i$ and $w_i = \mu(\mathbb{R})v_{i,0}^2$, where v_i is the ith column of V and $v_{i,0}$ is the first component of v_i.

Example 13. The **Hermite polynomials** $H_n(x)$, which are defined to have leading coefficient 2^n, result if $d\mu(x) := e^{-x^2}\,dx$. In particular, note that $\mu(\mathbb{R}) = \sqrt{\pi}$. Since the leading coefficient of H_n is 2^n, $\varphi_n(x) = H_n(x)/2^n$. The three-term recurrence for the H_n is well-known to be

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x),$$

where $H_0(x) = 1$. Dividing by 2^{n+1} yields

$$\frac{H_{n+1}(x)}{2^{n+1}} = x\frac{H_n(x)}{2^n} - \frac{n}{2}\frac{H_{n-1}(x)}{2^{n-1}},$$

or

$$\varphi_{n+1}(x) = (x-0)\varphi_n(x) - \frac{n}{2}\varphi_{n-1}(x).$$

Hence, $a_n = 0$ and $b_n = n/2$. The Hermite nodes and weights are easily generated with the following MATLAB function.

```
function [x,w] = hermitequad(n)
%
% Generate nodes and weights for
% Hermite-Gauss quadrature.
% Note that x is a column vector
% and w is a row vector.
%
u = sqrt([1:n-1]/2); % upper diagonal of J
[V,Lambda] = eig(diag(u,1)+diag(u,-1));
[x,i] = sort(diag(Lambda));
Vtop = V(1,:);
Vtop = Vtop(i);
w = sqrt(pi)*Vtop.^2;
```

Example 14. The **Laguerre polynomials** $L_n(x)$, which are defined to have leading coefficient $(-1)^n/n!$, result if $d\mu(x) := e^{-x}\,dx$ for $x \geq 0$. In particular, note that $\mu(\mathbb{R}) = 1$. Since the leading coefficient of L_n is $(-1)^n/n!$, $\varphi_n(x) = L_n(x)n!/(-1)^n$. The three-term recurrence for the L_n is well-known to be

$$(n+1)L_{n+1}(x) = (2n+1-x)L_n(x) - nL_{n-1}(x),$$

where $L_0(x) = 1$. A little algebra shows that

$$\varphi_{n+1}(x) = (x - [2n+1])\varphi_n(x) - n^2\varphi_{n-1}(x).$$

Hence, $a_n = 2n+1$ and $b_n = n^2$. The Laguerre nodes and weights are easily generated with the following MATLAB function.

```
function [x,w] = laguerrequad(n)
%
% Generate nodes and weights for
% Laguerre-Gauss quadrature.
% Note that x is a column vector
% and w is a row vector.
%
a = 2*[0:n-1]+1; % diagonal of J
u = [1:n-1]; % upper diagonal of J
[V,Lambda] = eig(diag(u,1)+diag(a)+diag(u,-1));
[x,i] = sort(diag(Lambda));
Vtop = V(1,:);
Vtop = Vtop(i);
w = Vtop.^2;
```

Example 15. The **Legendre polynomials** $P_n(x)$, which are defined to have leading coefficient $(2n)!/(2^n(n!)^2)$, result if $d\mu(x) := dx$ for $-1 \leq x \leq 1$. In particular, note that $\mu(\mathbb{R}) = 2$. Since the leading coefficient of P_n is $(2n)!/(2^n(n!)^2)$, $\varphi_n(x) = P_n(x)2^n(n!)^2/(2n)!$. The three-term recurrence for the P_n is well-known to be

$$(n+1)P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x),$$

where $P_0(x) = 1$. A little algebra shows that

$$\varphi_{n+1}(x) = (x-0)\varphi_n(x) - \frac{n^2}{4n^2-1}\varphi_{n-1}(x).$$

Hence, $a_n = 0$ and $b_n = 1/(4 - n^{-2})$. The Legendre nodes and weights are easily generated with the following MATLAB function.

```
function [x,w] = legendrequad(n)
%
% Generate nodes and weights for
```

```
% Legendre-Gauss quadrature on [-1,1].
% Note that x is a column vector
% and w is a row vector.
%
u = sqrt(1./(4-1./[1:n-1].^2)); % upper diag.
[V,Lambda] = eig(diag(u,1)+diag(u,-1));
[x,i] = sort(diag(Lambda));
Vtop = V(1,:);
Vtop = Vtop(i);
w = 2*Vtop.^2;
```

Example 16. The ***shifted*** **Legendre polynomials** are $P_n^*(x) := P_n(2x-1)$. The P_n^* have leading coefficient $(2n)!/(n!)^2$. These polynomials result if $d\mu(x) := dx$ for $0 \leq x \leq 1$. In particular, note that $\mu(\mathbb{R}) = 1$. Since the leading coefficient of P_n^* is $(2n)!/(n!)^2$, $\varphi_n(x) = P_n^*(x)(n!)^2/(2n)!$. The three-term recurrence for the P_n^* is easily seen to be

$$(n+1)P_{n+1}^*(x) = (2n+1)(2x-1)P_n^*(x) - nP_{n-1}^*(x),$$

where $P_0^*(x) = 1$. A little algebra shows that

$$\varphi_{n+1}(x) = (x-1/2)\varphi_n(x) - \frac{n^2}{4(4n^2-1)}\varphi_{n-1}(x).$$

Hence, $a_n = 1/2$ and $b_n = 1/(4(4-n^{-2}))$. The shifted Legendre nodes and weights are easily generated with the following MATLAB function.

```
function [x,w] = legendrequad01(n)
%
% Generate nodes and weights for shifted
% Legendre-Gauss quadrature on [0,1].
% Note that x is a column vector
% and w is a row vector.
%
a = repmat(1/2,1,n); % main diagonal of J
u = sqrt(1./(4*(4-1./[1:n-1].^2)));
[V,Lambda] = eig(diag(u,1)+diag(a)+diag(u,-1));
[x,i] = sort(diag(Lambda));
Vtop = V(1,:);
Vtop = Vtop(i);
w = Vtop.^2;
```

Remark. By Lemma 5, the weights of a Gaussian quadrature must be positive. However, when n is large, some weights can numerically evaluate to zero. The follwing lines can be added to the preceding MATLAB functions to detect this and remove the unusable weights and nodes before returning.

```
i = find(w>0);
w = w(i);
x = x(i);
nw = length(i);
if nw < n
  fprintf('%g zero weights detected.\n',n-nw)
end
```

The parameter `nw` can be added to the list of variables returned to the calling program so it can check if `nw` is less than `n`.

Theorem 17. *The weights and nodes of the Chebyshev, Legendre, and Hermite quadrature rules exhibit symmetry and antisymmetry, respectively.*

Proof. If one computes the first few orthogonal polynomials mentioned, one quickly sees that the even powers are even functions and the odd powers are odd functions. Hence, their roots have the property that if x is a root, then so is $-x$.

Using the antisymmetry of the nodes, we can show that the weights are symmetric using (2). For example, for $n = 6$, we can use the fact that $x_4 = -x_3$, $x_5 = -x_2$, and $x_6 = -x_1$ to write

$$\begin{aligned}\ell_2(x) &= \frac{(x-x_1)(x-x_3)(x-x_4)(x-x_5)(x-x_6)}{(x_2-x_1)(x_2-x_3)(x_2-x_4)(x_2-x_5)(x_2-x_6)} \\ &= \frac{(x^2-x_1^2)(x^2-x_3^2)}{(x_2^2-x_1^2)(x_2^2-x_3^2)} \cdot \frac{1}{2x_2} \cdot (x_2+x).\end{aligned}$$

Similarly,

$$\begin{aligned}\ell_5(x) &= \frac{(x-x_1)(x-x_2)(x-x_3)(x-x_4)(x-x_6)}{(x_5-x_1)(x_5-x_2)(x_5-x_3)(x_5-x_4)(x_5-x_6)} \\ &= \frac{(x^2-x_1^2)(x^2-x_3^2)}{(x_2^2-x_1^2)(x_2^2-x_3^2)} \cdot \frac{1}{2x_2} \cdot (x_2-x).\end{aligned}$$

Since $\ell_5(-x) = \ell_2(x)$ and since the weight functions for $d\mu$ are even, we see from (2) that $w_5 = w_2$. □

Proof of Theorem 12. The first step is to rewrite the three-term recurrence

$$\varphi_k(x) = (x-a_{k-1})\varphi_{k-1}(x) - b_{k-1}\varphi_{k-2}(x)$$

in terms of the ortho*normal* polynomials $\psi_k := \varphi_k/\|\varphi_k\|$. This leads to

$$\|\varphi_k\|\psi_k(x) = (x-a_{k-1})\|\varphi_{k-1}\|\psi_{k-1}(x) - b_{k-1}\|\varphi_{k-2}\|\psi_{k-2}(x).$$

Divide this equation by $\|\varphi_{k-1}\|$ and use the fact that $\sqrt{b_k} = \|\varphi_k\|/\|\varphi_{k-1}\|$ to obtain

$$\sqrt{b_k}\,\psi_k(x) = (x-a_{k-1})\psi_{k-1}(x) - \sqrt{b_{k-1}}\,\psi_{k-2}(x).$$

Rearrange this as

$$x\psi_{k-1}(x) = \sqrt{b_k}\,\psi_k(x) + a_{k-1}\psi_{k-1}(x) + \sqrt{b_{k-1}}\,\psi_{k-2}(x).$$

If we write out this formula for $k = 1, \ldots, n$, we get a system of n linear equations. To express this in matrix-vector notation, put

$$\Psi(x) := [\psi_0(x), \ldots, \psi_{n-1}(x)]'.$$

Then the system of linear equations can be written as

$$x\Psi(x) = J_n\Psi(x) + \begin{bmatrix} 0 \\ \vdots \\ 0 \\ \sqrt{b_n}\,\psi_n(x) \end{bmatrix}.$$

Now, if $x = x_i$ is the ith root of φ_n, which is also the ith root of $\psi_n = \varphi_n/\|\varphi_n\|$, then the matrix-vector equation reduces to

$$x_i\Psi(x_i) = J_n\Psi(x_i),$$

which says that x_i is an eigenvalue of J_n with eigenvector $\Psi(x_i)$. Since by definition eigenvectors cannot be the zero vector, we should check this condition. By (9), $(\sqrt{w_i}\Psi(x_i))'(\sqrt{w_i}\Psi(x_i)) = 1$. Hence, $\sqrt{w_i}\Psi(x_i)$ is a unit-norm eigenvector of J_n. Since we are working in a real vector space, $\sqrt{w_i}\Psi(x_i)$ must be equal to plus or minus the ith column vector of V. Since $\sqrt{w_i}\Psi(x_i) = \pm v_i$, their first components must obey this relation too. Since the first component of $\Psi(x_i)$ is $\psi_0(x_i) = 1/\|\varphi_0\|$, the theorem is proved. □

Remark. An easy corollary of this theorem is that

$$\varphi_n(x) = \det(xI - J_n). \tag{11}$$

The right-hand side is a polynomial of degree n with leading coefficient one and whose roots are the eigenvalues of J_n. Hence, the right-hand side is exactly $(x-x_1)\cdots(x-x_n) = \varphi_n(x)$. An alternative way to prove (11) is the expand the determinant along the last column of $xI - J_n$ to show that $\det(xI - J_n)$ satisfies the same three-term recurrence as φ_n; hence, $\det(xI - J_n) = \varphi_n(x)$.

According to Gautschi [1], the fact that the roots of φ_n are the eigenvalues of J_n was known prior to the 1960s. The relationship of the weights to the *orthonormal* eigenvectors of J_n is found in Wilf [8, Ch. 2, Ex. 9]. Gautschi also says that this fact was known to Goertzel around 1954 and appeared in Gordon [4] in 1968. It was Golub and Welsch [3] who provided an efficient algorithm for solving the eigenvalue problem for J_n to obtain the eigenvalues x_i and the weights w_i.

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