10. Gaussian Quadrature

10.1. **Quadrature formulas with given abscissas.** We have previously seen that one way of obtaining quadrature formulas of the form

$$\int_a^b f(x)\,dx = \sum_{j=0}^n H_j f(x_j) + E$$

in the case when the x_j are specified is to integrate the polynomial of degree $\le n$ interpolating f at the points $x_0, \cdots, x_n$. Abstractly, we could use the Lagrange form of the interpolating polynomial, $P_n(x) = \sum_{j=0}^n L_{j,n}(x) f(x_j)$ to obtain the formula

$$\int_a^b f(x)\,dx \approx \int_a^b P_n(x)\,dx = \sum_{j=0}^n \left[\int_a^b L_{j,n}(x)\,dx\right] f(x_j),$$

i.e., $H_j = \int_a^b L_{j,n}(x)\,dx$. (In our derivations, we used the Newton form of the interpolating polynomial.)

When f is a polynomial of degree $\le n$, $f \equiv P_n$, so the quadrature formula is exact for all polynomials of degree $\le n$. Hence, we have determined quadrature formulas of the above form, where the H_j are determined by the criteria that the formula be exact for polynomials of as high a degree as possible. We could also obtain these formulas by the method of undetermined coefficients. Since we have $n+1$ weights H_j, we would expect exactness for polynomials of degree $\le n$. Substituting $f(x) = x^k$, $k = 0, \cdots, n$, we get the equations:

$$\int_a^b x^k\,dx = \sum_{j=0}^n H_j x_j^k.$$

This is a set of $n+1$ linear equations for $H_0, \cdots, H_n$.

$$\begin{pmatrix} 1 & 1 & \cdots & 1 \\ x_0 & x_1 & \cdots & x_n \\ \cdots & \cdots & \cdots & \cdots \\ x_0^n & x_1^n & \cdots & x_n^n \end{pmatrix} \begin{pmatrix} H_0 \\ H_1 \\ \cdots \\ H_n \end{pmatrix} = \begin{pmatrix} b-a \\ (b^2-a^2)/2 \\ \cdots \\ (b^{n+1}-a^{n+1})/(n+1) \end{pmatrix}$$

This matrix is the transpose of the Vandermonde matrix and hence is nonsingular. So the H_js are uniquely determined.

Note that if these equations hold, then if $P_n(x) = \sum_{k=0}^n c_k x^k$,

$$\int_a^b P_n(x)\,dx = \sum_{k=0}^n c_k \int_a^b x^k\,dx = \sum_{k=0}^n c_k \sum_{j=0}^n H_j x_j^k = \sum_{j=0}^n H_j \sum_{k=0}^n c_k x_j^k = \sum_{j=0}^n H_j P_n(x_j),$$

so the formula is exact for all polynomials of degree $\le n$.

We can also consider the x_js as unknowns and try to determine both the x_j and H_j to make the resulting quadrature formula exact for as high degree polynomials as possible. Such formulas are called Gaussian quadrature formulas.

10.2. **Gaussian quadrature formulas.** If we try the method of undetermined coefficents to get such formulas, we obtain the equations

$$\int_a^b x^k\,dx = (b^{k+1} - a^{k+1})/(k+1) = \sum_{j=0}^{n} H_j x_j^k, \qquad k = 0, 1, \ldots.$$

There are now $2n+2$ unknowns, so we could take $2n+2$ equations. However, the equations are now nonlinear, so it is not clear whether this system will have a solution, and even if it does, obtaining the solution is not simple.

We instead use a different approach using the idea of orthogonal polynomials. It is convenient to consider a slightly more general problem, i.e., we introduce a fixed weight function $w(x)$ and look for a formula of the form

$$\int_a^b w(x) f(x)\,dx = \sum_{j=0}^{n} H_j f(x_j) + E.$$

We assume that $w(x)$ is continuous on (a, b) and $w(x) > 0$, except at most a set of isolated values. The advantages of this formulation and special choices of $w(x)$ will be discussed later. Obviously, $w(x) \equiv 1$ reduces to the original problem. We also allow a and b to be infinite, as well as finite.

10.3. **Orthogonal polynomials.** Define $(f, g) = \int_a^b w(x) f(x) g(x)\,dx$. One can show that $(\cdot, \cdot)$ is an inner product on the space

$$V = \{f : f \in C^0(a, b), \int_a^b w(x) f^2(x)\,dx < \infty\}.$$

That is, we have the properties:

$$(f, g) = (g, f), \qquad (f + g, h) = (f, h) + (g, h), \qquad (\lambda f, g) = \lambda(f, g), \quad \lambda \in \mathbb{R},$$
$$(f, f) \geq 0, \qquad (f, f) = 0 \iff f = 0.$$

We can also define the norm of f, $\|f\| = \sqrt{(f, f)}$.

We say f and g are othogonal if $(f, g) = 0$. Then a set $f_1, \cdots, f_n$ is an orthogonal set of functions if $(f_i, f_j) = 0$, $i \neq j$. A set $f_1, \cdots, f_n$ is orthonormal if $f_1, \cdots, f_n$ is orthogonal and $(f_i, f_i) = 1, i = 1, \ldots, n$.

In the following discussion, we let $\Phi_0(x), \Phi_1(x), \cdots$ be a set of polynomials satisfying (i) $\Phi_j(x)$ is of degree j and (ii) $(\Phi_j, \Phi_k) = 0$, $j \neq k$ (i.e., we have a set of orthogonal polynomials).

Properties of orthogonal polynomials:

Lemma 3. *A non-zero polynomial $P(x)$ of degree at most k is orthogonal to every polynomial of degree $< k$ if and only if $P(x) = c\Phi_k(x)$ for some non-zero constant c.*

Proof. Let $P(x) = c\Phi_k(x)$. We first show that $(P, Q) = 0$ for any polynomial $Q(x)$ of degree $< k$. To do so, we observe that any set of $j+1$ polynomials of exact degrees $0, 1, \ldots, j$ is a basis for the set of all polynomials of degree $\leq j$. Hence, any polynomial $Q(x)$ of degree

$< k$ is a linear combination of $\Phi_0, \Phi_1, \ldots, \Phi_{k-1}$. Since Φ_k is orthogonal to each of these by assumption, it is orthogonal to Q and hence $(P, Q) = 0$.

Now assume $P(x)$ of degree at most k is orthogonal to every polynomial of degree $< k$. Then for any constant c, so is $P(x) - c\Phi_k(x)$. Choose c so that the coefficient of x^k in $P(x) - c\Phi_k(x)$ is equal to zero. For this value of c, $R(x) = P(x) - c\Phi_k(x)$ is of degree $< k$. Hence, $R(x)$ is orthogonal to itself, so $R(x) \equiv 0$, i.e., $P(x) = c\Phi_k(x)$. □

Corollary: Orthogonal polynomials are unique to within multiplication by non-zero constants. Hence, we still have a set of arbitrary constants to specifiy to completely determine a set of orthogonal polynomials. We use these constants to normalize the polynomials in some convenient way. Two standard possibilities: (i) make the leading coefficient (of x^k) in $\Phi_k(x)$ equal to one or (ii) make $\|\Phi_k\| = 1$, i.e., make the set orthonormal.

Remark: We are assuming a fixed inner product. If the weight function $w(x)$ or the limits of integration a or b are changed, then we have a new inner product and hence a new set of orthogonal polynomials.

Using Lemma 3, we now prove a key result for the derivation of the quadrature formula.

Theorem 6. *$\Phi_k(x)$ has k real distinct zeroes lying in (a, b).*

Proof. Let $a_1, \ldots, a_k$ be the roots of $\Phi_k(x)$. As x varies from a to b, let $\Phi_k(x)$ change sign at the points $b_1, \ldots, b_l$. Obviously, $\Phi_k(b_j) = 0$ and so the b_j are a subset of the a_j $(l \le k)$. Let $P(x) = \prod_{j=1}^{l}(x - b_j)$ if $l \ge 1$, $P(x) \equiv 1$ if $l = 0$. Now $P(x)$ also changes sign at $b_1, \ldots b_l$ since one factor changes sign as x crosses b_j. Hence, $P(x)\Phi_k(x)$ is either always ≥ 0 or always ≤ 0. Since $w(x) > 0$,

$$(P, \Phi_k) = \int_a^b w(x)P(x)\Phi_k(x)\,dx \neq 0.$$

By Lemma 3, the degree of $P(x)$ is at least k, i.e., $l = k$ and $a_1, \cdots, a_k = b_1, \cdots, b_k$ are distinct real zeroes of $\Phi_k(x)$. □

We next present an algorithm for the construction of a set of orthogonal polynomials (for a given inner product).

Theorem 7. *Lanczo's Orthogonalization theorem Let*

$$\Phi_0 = 1, \qquad \Phi_1 = x - \alpha_1, \qquad \Phi_k = x\Phi_{k-1} - \alpha_k\Phi_{k-1} - \beta_k\Phi_{k-2}, \quad k = 2, 3, \cdots,$$

where

$$\gamma_k = (\Phi_k, \Phi_k), \quad k = 0, 1, \ldots, \qquad \alpha_k = (x\Phi_{k-1}, \Phi_{k-1})/\gamma_{k-1}, \quad k = 1, 2, \ldots,$$
$$\beta_k = (x\Phi_{k-1}, \Phi_{k-2})/\gamma_{k-2}, \quad k = 2, 3, \ldots.$$

Then $\Phi_0, \Phi_1, \ldots$ are an orthogonal set of polynomials.

Proof. We need to prove the following: For $k = 0, 1, \cdots$, (i) Φ_k is a polynomial of degree k, (ii) $\gamma_k \neq 0$, since we must divide by it, and (iii) $(\Phi_k, \Phi_j) = 0$ for $j < k$. Now (ii) follows from (i), since if Φ_k is a polynomial of degree k, it cannot be zero and hence $\gamma_k \neq 0$. We now prove (i) and (iii) by induction.

$k = 0$. Φ_0 is of degree zero. Since there is no $j < 0$, (iii) is not applicable. $\gamma_0 = (1, 1)$.

$k = 1$. Φ_1 is of degree one. $\alpha_1 = (x, 1)/(1, 1)$ and

$$(\Phi_1, \Phi_0) = (x - \alpha_1, 1) = (x, 1) - \alpha_1(1, 1) = 0.$$

Now assume (i), (ii), and (iii) hold for all Φ_l with $l < k$. We will show that (i) and (iii) hold for $l = k$. Now $\Phi_k = x\Phi_{k-1} - \alpha_k\Phi_{k-1} - \beta_k\Phi_{k-2}$. Since Φ_{k-1} and Φ_{k-2} are of degrees $k-1$ and $k-2$, respectively, $x\Phi_{k-1}$ is of degree k and hence Φ_k is of degree k. This establishes (i). The proof of (iii) requires three cases ($j = k-1$, $j = k-2$, $j < k-2$). Now

$$(\Phi_k, \Phi_{k-1}) = (x\Phi_{k-1}, \Phi_{k-1}) - \alpha_k(\Phi_{k-1}, \Phi_{k-1}) - \beta_k(\Phi_{k-2}, \Phi_{k-1}) = 0$$

using the definition of α_k and the fact that (iii) holds for $l = k-1$, i.e., $(\Phi_{k-2}, \Phi_{k-1}) = 0$. When $j = k-2$,

$$(\Phi_k, \Phi_{k-2}) = (x\Phi_{k-1}, \Phi_{k-2}) - \alpha_k(\Phi_{k-1}, \Phi_{k-2}) - \beta_k(\Phi_{k-2}, \Phi_{k-2}) = 0$$

using the definition of β_k and the fact that (iii) holds for $l = k-1$, i.e., $(\Phi_{k-2}, \Phi_{k-1}) = 0$. Finally, when $j < k-2$,

$$\begin{aligned}(\Phi_k, \Phi_j) &= (x\Phi_{k-1}, \Phi_j) - \alpha_k(\Phi_{k-1}, \Phi_j) - \beta_k(\Phi_{k-2}, \Phi_j) \\ &= (\Phi_{k-1}, x\Phi_j) - \alpha_k(\Phi_{k-1}, \Phi_j) - \beta_k(\Phi_{k-2}, \Phi_j).\end{aligned}$$

Since $x\Phi_j$ is of degree $< k-1$, we again use the fact that (iii) holds for $k-1$ and $k-2$ to conclude that all terms on the right hand side are equal to zero. □

Corollary 2: The leading term of Φ_k has coefficient one.

Corollary 3: $\beta_k = \gamma_{k-1}/\gamma_{k-2}$.

$$\begin{aligned}\gamma_{k-2}\beta_k = (x\Phi_{k-1}, \Phi_{k-2}) &= (\Phi_{k-1}, x\Phi_{k-2}) \\ &= (\Phi_{k-1}, \Phi_{k-1}) + \alpha_{k-1}(\Phi_{k-1}, \Phi_{k-2}) + \beta_{k-1}(\Phi_{k-1}, \Phi_{k-3}) = \gamma_{k-1}.\end{aligned}$$

Corollary 4: $\gamma_k = (x^k, \Phi_k)$.

$$\gamma_k = (\Phi_k, \Phi_k) = (x^k + P(x), \Phi_k) = (x^k, \Phi_k),$$

using Lemma 3 and the fact that $P(x)$ is a polynomial of degree at most $k-1$.

Corollary 5: If $\Phi_{k-1}(x) = x^{k-1} + c_{k-1}x^{k-2} + \cdots +$, then $\alpha_k = (x^k, \Phi_{k-1})/\gamma_{k-1} + c_{k-1}$.

$$\begin{aligned}\alpha_k &= (x\Phi_{k-1}, \Phi_{k-1})/\gamma_{k-1} = (x[x^{k-1} + c_{k-1}x^{k-2} + \cdots +], \Phi_{k-1})/\gamma_{k-1} \\ &= (x^k, \Phi_{k-1})/\gamma_{k-1} + c_{k-1}(x^{k-1}, \Phi_{k-1})/\gamma_{k-1} + 0 = (x^k, \Phi_{k-1})/\gamma_{k-1} + c_{k-1}.\end{aligned}$$

Remark: Corollaries 3, 4, and provide the most convenient formulas for constucting the orthogonal polynomials.