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 $P_n(x) = \sum_{k=0}^{n} c_k x^k$,

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

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 coefficients 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. For example, when $n = 1$, we seek to determine x_0, x_1, H_0, H_1 satisfying:

$$b - a = H_0 + H_1, \qquad (b^2 - a^2)/2 = H_0 x_0 + H_1 x_1 \qquad (b^3 - a^3)/3 = H_0 x_0^2 + H_1 x_1^2,$$
$$(b^4 - a^4)/4 = H_0 x_0^3 + H_1 x_1^3.$$

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 orthogonal 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).

Algorithm for constructing a set of orthogonal polynomials (for a given inner product):

Theorem 10. *(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

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

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

Remark: In general, orthogonal polynomials are unique to within multiplication by non-zero constants, so you may find slightly different variations in other sources.

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.

Example: $a = -1$, $b = 1$, $w = 1$, $\Phi_0(x) = 1$, $\Phi_1(x) = x$, $\Phi_2(x) = x^2 - 1/3$.

A key property of orthogonal polynomials is the following.

Lemma 2. *$\Phi_k(x)$ has k real distinct zeroes lying in (a, b).*

10.4. **Construction of Gaussian quadrature formulas.** Our main result is the following theorem.

Theorem 11. *There exist abscissas $x_0, \cdots, x_n$ and weights $H_0, \cdots, H_n$ such that*

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

for all polynomials $P(x)$ of degree $\leq 2n+1$ if and only if the x_j are the zeroes of Φ_{n+1}. Then the constants H_j are given by the formula

$$H_j = \int_a^b w(x) L_{j,n}(x)\, dx, \qquad \text{where} \qquad L_{j,n}(x) = \prod_{\substack{i=0 \\ i \neq j}}^{n} (x - x_i)/(x_j - x_i).$$

Example: $a = -1$, $b = 1$, $w = 1$, $n = 1$, x_0, x_1 roots of $\Phi_2 = x^2 - 1/3$, i.e., $\pm 1/\sqrt{3}$. Then

$$H_0 = \int_{-1}^{1} \frac{x - 1/\sqrt{3}}{-1/\sqrt{3} - 1/\sqrt{3}}\, dx = 1, \qquad H_0 = \int_{-1}^{1} \frac{x + 1/\sqrt{3}}{1/\sqrt{3} + 1/\sqrt{3}}\, dx = 1.$$

We next derive a formula for the error in this approximation.

Theorem 12. *If the x_j and H_j are defined as in Theorem (11), and if $f(x) \in V$ satisfies $f^{(2n+2)}$ is continuous in (a, b), then for some $\xi \in (a, b)$,*

$$E = \int_a^b f(x)\, dx - \sum_{j-0}^{n} H_j f(a_j) = \frac{\gamma_{n+1}}{(2n+2)!} f^{(2n+2)}(\xi).$$

Proof. Denote by $Q(x)$ the polynomial of degree $\leq 2n+1$ which solves the Hermite interpolation problem $Q(x_i) = f(x_i)$, $Q'(x_i) = f'(x_i), i = 0, \ldots, n$. By Theorem (11), the Gauss quadrature formula is exact for $Q(x)$, i.e.,

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

Hence, by the error formula for polynomial interpolation,

$$\begin{aligned} E &= \int_a^b w(x)f(x)\,dx - \sum_{j=0}^n H_j f(x_j) = \int_a^b w(x)[f(x) - Q(x)]\,dx \\ &= \int_a^b w(x) f[x_0, x_0, x_1, x_1, \cdots, x_n, x_n, x] \prod_{j=0}^n (x - x_j)^2\,dx \\ &= \frac{f^{(2n+2)}(\xi_x)}{(2n+2)!} \int_a^b w(x) \prod_{j=0}^n (x - x_j)^2\,dx = \frac{f^{(2n+2)}(\xi_x)}{(2n+2)!} \int_a^b w(x)\Phi_{n+1}^2(x)\,dx, \end{aligned}$$

where we have used the fact that Φ_{n+1} is the unique polynomial of degree n with leading coefficient equal to one, with zeros at $x_0, \ldots, x_n$. $\square$

Example: Example: $a = -1$, $b = 1$, $w = 1$, $n = 1$.

$$\gamma_2 = (x^2, \Phi_2) = \int_{-1}^1 x^2(x^2 - 1/3)\,dx = 8/45, \qquad E = \frac{\gamma_{n+1}}{(2n+2)!} f^{(2n+2)}(\xi) = \frac{8/45}{(4)!} f^{(4)}(\xi).$$

10.5. **Examples of orthogonal polynomials.** We next present standard sets of orthogonal polynomials corresponding to different choices of weight functions $w(x)$ and limits of integration a and b.

(i) $a = -1, b = 1, w(x) \equiv 1$. Legendre polynomials. The corresponding quadrature formula is called the Legendre-Gauss quadrature formula.

(ii) $a = 0, b = \infty, w(x) = e^{-x}$. Laguerre polynomials.

(iii) $a = -1, b = 1, w(x) = 1/\sqrt{1-x^2}$. Chebyshev polynomials.

(iv) $a = -\infty, b = \infty, w(x) = e^{-x^2}$. Hermite polynomials.

There are several advantages to including a weight function $w(x)$. When either or both a and b are infinite, it is convenient to choose $w(x)$ to insure convergence of the integral of $w(x)f(x)$, where $f(x)$ is a polynomial of arbitrary degree (as in (ii) and (iii) above). In singular integrals, e.g., with terms like $1/\sqrt{1-x^2}$, it is convenient to have formulas and error terms that do not depend on these terms.