9 Gauss quadrature and orthogonal polynomials.

The aim of this section is to construct "optimal" quadrature formulas. To be more specific, given the integral

$$I_w(f) = \int_a^b w(x)f(x)dx \tag{32}$$

in which $w(x)$ is a fixed, positive function. We want to approximate this using a quadrature formula on the form

$$Q_w(f) = \sum_{i=1}^{n} A_i f(x_i).$$

Such a formula can be constructed as follows: Choose n distinct nodes, $x_1, x_2, \cdots, x_n$ in the interval $[a, b]$. Construct the interpolation polynomial

$$p_{n-1}(x) = \sum_{i=1}^{n} f(x_i)\ell_i(x), \qquad \ell_i(x) = \prod_{j=1, j\neq i} \frac{x - x_j}{x - x_i}.$$

An approximation to the integral is then given by

$$Q_w(f) = \int_a^b w(x)p_{n-1}(x)dx = \sum_{i=1}^{m} A_i f(x_i), \qquad A_i = \int_a^b w(x)\ell_i(x)dx. \tag{33}$$

The quadrature formula is of precision m if

$$I_w(p) = Q_w(p), \qquad \text{for all } p \in \mathbb{P}_m.$$

From the construction, these quadrature formulas is of precision at least $n - 1$. The question is how too choose the nodes x_i, $i = 1, \ldots, n$ giving m as large as possible. The key concept here is *orthogonal polynomials.*

Orthogonal polynomials.

Given two functions $f, g \in C[a, b]$. We define an inner product of these two functions by

$$< f, g >= \int_a^b w(x)f(x)g(x)dx, \qquad w(x) > 0. \tag{34}$$

Thus the definition of the inner product depends on the integration interval $[a, b]$ and a given *weight function* $w(x)$. If $f, g, h \in C[a, b]$ and $\alpha \in \mathbb{R}$ then

$$\begin{aligned}
\langle f, g\rangle_w &= \langle g, f\rangle_w \\
\langle f + g, h\rangle_w &= \langle f, h\rangle_w + \langle g, h\rangle_w \\
\langle \alpha f, g\rangle_w &= \alpha\langle f, g\rangle_w \\
\langle f, f\rangle_w &\geq 0, \qquad \text{and} \qquad \langle f, f\rangle_w = 0 \Leftrightarrow f \equiv 0.
\end{aligned}$$

From an inner product, we can also define a norm on $C[a, b]$ by

$$\|f\|_w^2 = \langle f, f\rangle_w.$$

For the inner product (34) we also have

$$\langle xf, g\rangle_w = \int_a^b w(x)xf(x)g(x)dx = \langle f, xg\rangle_w. \qquad (35)$$

Our aim is now to create an orthogonal basis for $\mathbb{P}$, that is, create a sequence of polynomials $\phi_k(x)$ of degree k (no more, no less) for $k = 0, 1, 2, 3, \ldots$ such that

$$\langle \phi_i, \phi_j\rangle_w = 0 \quad \text{for all} \quad i \neq j.$$

If we can make such a sequence, then

$$\mathbb{P}_{n-1} = \text{span}\{\phi_0, \phi_1, \cdots, \phi_{n-1}\} \qquad \text{and} \qquad \langle \phi_n, p\rangle_w = 0 \quad \text{for all} \qquad p \in \mathbb{P}_{n-1}.$$

Let us now find the sequence of orthogonal polynomials. This is done by a Gram-Schmidt process:

Let $\phi_0 = 1$. Let $\phi_1 = x - B_1\phi_0$ where B_1 is given by the orthogonality condition:

$$0 = \langle \phi_1, \phi_0\rangle_w = \langle x\phi_0, \phi_0\rangle_w - B_1\langle \phi_0, \phi_0\rangle_w \qquad \Rightarrow \qquad B_1 = \frac{\langle x\phi_0, \phi_0\rangle_w}{\|\phi_0\|_w^2}.$$

Let us now assume that we have found ϕ_j, $j = 0, 1, \cdots, \phi_k$. Then, let

$$\phi_k = x\phi_{k-1} - \sum_{j=0}^{k-1} \alpha_j\phi_j.$$

Clearly, ϕ_k is a polynomial of degree k, and α_j can be chosen so that $\langle \phi_k, \phi_i\rangle_w = 0$, $i = 0, 1, \ldots, k-1$, or

$$\langle \phi_k, \phi_i\rangle_w = \langle x\phi_{k-1}, \phi_i\rangle_w - \sum_{j=0}^{k-1} \alpha_j\langle \phi_i, \phi_j\rangle_w = \langle x\phi_{k-1}, \phi_i\rangle_w - \alpha_i\langle \phi_i, \phi_i\rangle_w = 0, \qquad i = 0, 1, \cdots, k-1.$$

So $\alpha_i = \langle x\phi k - 1, \phi_i\rangle_w / \langle \phi_i, \phi_i\rangle_w$. But we can do even better. Since ϕ_{k-1} is orthogonal to all polynomials of degree $k-2$ or less, we get

$$\langle x\phi_{k-1}, \phi_i\rangle_w = \langle \phi_{k-1}, x\phi_i\rangle_w = 0 \quad \text{for} \quad i + 1 < k - 1.$$

So, we are left only with α_{k-1} and α_{k-2}. The following theorem concludes the argument:

Theorem 9.1. *The sequence of orthogonal polynomials can be defined as follows:*

$$\phi_1(x) = 1, \qquad \phi_2(x) = x - B_1$$
$$\phi_k(x) = (x - B_k)\phi_{k-1}(x) - C_k\phi_{k-2}(x), \qquad k \geq 2$$

with

$$B_k = \frac{\langle x\phi_{k-1}, \phi_{k-1}\rangle_w}{\|\phi k - 1\|_w^2}, \qquad C_k = \frac{\langle x\phi_{k-1}, \phi_{k-2}\rangle_w}{\|\phi_{k-2}\|_w^2} = \frac{\|\phi_{k-1}\|_w^2}{\|\phi_{k-2}\|_w^2}$$

The last simplification of C_k is given by:

$$\langle x\phi_{k-1}, \phi_{k-2}\rangle_w = \langle \phi_{k-1}, x\phi_{k-2}\rangle_w$$
$$\phi_{k-1} = x\phi_{k-2} - B_{k-1}\phi_{k-2} - C_{k-1}\phi_{k-3}.$$

Solve the second with respect to $x\phi_{k-2}$, replace it into the right hand side of the first expression, and use the orthogonality conditions.

For the inner product

$$\langle f, g\rangle = \int_{-1}^{1} f(x)g(x)dx$$

we get the well known *Legendre polynomials*,

$$\begin{aligned} P_0(x) &= 1 \\ P_1(x) &= x \\ P_2(x) &= x^2 - \frac{1}{3} \\ P_3(x) &= x^3 - \frac{3}{5}x \\ &\vdots \end{aligned}$$

see Burden and Faires, sec. 8.2.

Example 9.2. *Let $w(x) = 1/\sqrt{(1-x^2}$, and $[a,b] = [-1,1]$. We then get the sequence of polynomials:*

$$\begin{array}{lllll} \phi_0 = 1, & \langle x\phi_0, \phi_0\rangle_w = 0, & \langle \phi_0, \phi_0\rangle_w = \pi, & B_1 = 0, & \\ \phi_1 = x, & \langle x\phi_1, \phi_1\rangle_w = 0, & \langle \phi_1, \phi_1\rangle_w = \frac{\pi}{2}, & B_2 = 0, & C_2 = \frac{1}{2} \\ \phi_2 = x^2 - \frac{1}{2} & \langle x\phi_2, \phi_2\rangle_w = 0, & \langle \phi_2, \phi_2\rangle_w = \frac{\pi}{2}, & B_3 = 0, & C_3 = \frac{1}{4} \\ \phi_3 = x^3 - \frac{3}{4}x, & \quad etc. & & & \end{array}$$

These are nothing but the monic Chebyshev polynomials $\tilde{T}_k$ (see Burden and Faires, sec. 8.2).

The following theorem will become useful:

Theorem 9.3. *Let $f \in C[a,b]$, $f \not\equiv 0$ satisfying $\langle f, p\rangle_w = 0$ for all $p \in P_{k-1}$. Then f changes signs at least k times on (a,b).*

Proof. By contradiction. Suppose that f changes sign only $r < k$ times, at the points $t_1 < t_2 < \cdots < t_r$. Then f will not change sign on each of the subintervals:

$$(a, t_1), (t_1, t_2), \cdots, (t_{r-1}, t_r), (t_r, b).$$

Let $p(x) = \prod_{i=1}^{r}(x - t_i) \in \mathbb{P}_r \subseteq \mathbb{P}_{k-1}$. Then $p(x)$ has the same sign properties as $f(x)$, and $f(x)p(x)$ does Lt change sign on the interval. Since $w > 0$ we get

$$\int_a^b w(x)f(x)p(x) \neq 0$$

which contradicts the assumption of the theorem. □

Corollary 9.4. *The orthogonal polynomial ϕ_k has exactly k distinct zeros in (a,b).*

Gaussian quadrature

The main result of this section is the following result:

Theorem 9.5. *Let ϕ_n be the orthogonal polynomial of degree n based on the inner product* (34). *Let $x_1, x_2, \cdots, x_n$ be the distinct zeros of ϕ_n. Using these as nodes, the quadrature formula constructed by* (33) *is of precision* $2n-1$.

Proof. Let $p \in \mathbb{P}_{2n-1}$. By polynomial division with ϕ_n we get

$$p = q\phi_n + r, \qquad q, r \in \mathbb{P}_{n-1}.$$

By orthogonality, we get

$$I_w(p) = \int_a^b w(x)p(x)dx = \int_a^b w(x)q(x)\phi_n(x)dx + \int_a^b w(x)r(x)dx = \int_a^b w(x)r(x)dx = I_w(r)$$

And, since the nodes are zeros of ϕ_n we get

$$Q_w(p) = \sum_{i=1}^n A_i p(x_i) = \sum_{i=1}^n A_i q(x_i)\phi_n(x_i) + \sum_{i=1}^n A_i r(x_i) = Q_w(r).$$

But by construction $Q_w(f)$ has precision at least $n-1$, so $Q_w(r) = I_w(r)$. □

For Gaussian quadratures it is possible to prove that, for $f \in C^{2n}[a,b]$ we get

$$I_w(f) = Q_w(f) + E \tag{36}$$

with

$$E = \frac{f^{(2n)}(\nu)}{(2n)!}\int_a^b w(x)\omega(x)^2 dx, \qquad \omega(x) = \prod_{i=1}^n (x - x_i), \qquad \nu \in (a,b).$$

Example 9.6. *Let $w(x) = 1$ and $[a,b] = [-1,1]$, giving the Legendre polynomials as orthogonal polynomials. Choose e.g. $n = 3$, so that*

$$P_3(x) = x^3 - \frac{3}{5}x.$$

The zeros is $x_1 = -\sqrt{3/5}$, $x_2 = 0$ and $x_3 = \sqrt{3/5}$. From (33) *we get $A_1 = A_3 = 5/9$, $A_2 = 8/9$, so*

$$Q(f) = \frac{1}{9}\big(5f(x_1) + 8f(x_0) + 5f(x_2)\big). \tag{37}$$

The error of this formula becomes

$$E = \frac{f^{(6)}(\nu)}{15750}.$$

a) *Let us apply* (37) *to the integral*

$$\int_{-1}^1 e^x dx = 2.350402387.$$

This gives

$$\frac{1}{9}\big(5e^{-\sqrt{3/5}} + 8e^0 + 5e^{\sqrt{3/5}}\big) = 2.350336929$$

giving an error on $6.54 \cdot 10^{-5}$.

b) *Using the same formula on*

$$\int_{-1}^{1} \frac{e^x}{\sqrt{1-x^2}} dx = 3.977463261$$

gives $Q(f) = 3.199641132$ *which is a rather crude approximation. The reason is that* $f^{(2n)}(x) \to \infty$ *for* $x \to \pm 1$ *in this example.*

Example 9.7. *Let* $w(x) = 1/\sqrt{(1-x^2)}$ *and* $[a,b] = [-1,1]$, *giving the Chebyshev polynomials as orthogonal basis. Choose* $n = 3$, *so that*

$$\tilde{T}_3(x) = x^3 - \frac{3}{4}x,$$

with zeros $x_1 = -\sqrt{3}/2$, $x_2 = 0$ *and* $x_3 = \sqrt{3}/2$. *The corresponding weights becomes* $A_1 = A_2 = A_3 = \pi/3$, *and*

$$Q_w(f) = \frac{\pi}{3}\big(f(_1) + f(x_2) + f(x_3)\big).$$

The formula applied to the integral $\int_{-1}^{1} e^x/\sqrt{1-x^2}dx$ *is*

$$Q_w(e^x) = \frac{\pi}{3}\big(e^{-\sqrt{3}/2} + e^0 + e^{\sqrt{3}/2}\big) = 3.97732196$$

which is an significant improvement from the result of Example 9.6.b).