Gaussian Quadrature

Aim - compute

$$I[f] := \int_a^b w(x) f(x)\, dx$$

to prescribed accuracy.

$$I[f] \approx \int_a^b w(x)\, p_n(x)\, dx =: G_n[f]$$

$p_n(x)$ - Lagrange interpolation polynomial for f of degree n with interpolation points $x_0, \ldots, x_n$ as the roots of φ_{n+1}, the orthogonal polynomial of degree $n+1$.

$$G_n[f] = \int_a^b w(x) \{ L_0(x) f(x_0) + \ldots + L_n(x) f(x_n) \} dx$$

$$= \underbrace{\left[\int_a^b w(x) L_0(x)\, dx \right]}_{w_0} f(x_0) + \ldots + \underbrace{\left[\int_a^b w(x) L_n(x)\, dx \right]}_{w_n} f(x_n)$$

$$\boxed{L_k(x) = \prod_{\substack{j=1 \\ j \neq k}}^{n} \frac{(x - x_j)}{(x_k - x_j)}}$$

Use of roots of φ_{n+1} is motivated for instance by minimizing the interpolation error.

Ex

Consider $\int_{-1}^{1} \frac{1}{\sqrt{1-x^2}} f(x)\,dx.$

Find $G_1[f]$.

Corresponding orthogonal polynomials,
Chebyshev polynomials $T_n(x) = \cos(n.\arccos(x))$

$T_0(x) \equiv 1 \quad T_1(x) = x \quad T_2(x) = 2x\,T_1(x) - T_0(x) = 2x^2 - 1$

$x_0 = -1/\sqrt{2} \qquad x_1 = 1/\sqrt{2} \qquad \left(\begin{matrix}\text{roots of}\\ T_2(x)\end{matrix}\right)$

Weights

$$w_0 = \int_{-1}^{1} \frac{1}{\sqrt{1-x^2}} \frac{(x - 1/\sqrt{2})\,dx}{(-1/\sqrt{2} - 1/\sqrt{2})}$$

$$\overset{(x=\cos\theta)}{=} \int_{\pi}^{0} \frac{1}{\sqrt{1-\cos^2\theta}} \frac{(\cos\theta - 1/\sqrt{2})(-\sin\theta)\,d\theta}{(-\sqrt{2})}$$

$$= \int_{0}^{\pi} \frac{\cos\theta - 1/\sqrt{2}}{-\sqrt{2}}\,d\theta = \pi/2$$

$$w_1 = \int_{-1}^{1} \frac{1}{\sqrt{1-x^2}} \frac{(x + 1/\sqrt{2})}{(1/\sqrt{2} + 1/\sqrt{2})}\,dx$$

$$\boxed{G_1[f] = \frac{\pi}{2} f\left(\frac{-1}{\sqrt{2}}\right) + \frac{\pi}{2} f\left(\frac{1}{\sqrt{2}}\right)}$$

$$= \int_{0}^{\pi} \frac{\cos\theta + 1/\sqrt{2}}{\sqrt{2}}\,d\theta = \pi/2$$

THM (Optimality of Gaussian Quadrature)

(1) $I_n[f] = G_n[f] \quad \forall f \in \mathcal{P}_{2n+1}$

(2) There does not exist a quadrature formula (based on Lagrange interpolation $f(x_j) = p_n(x_j)$ at some interpolation points $x_0, x_1, \ldots, x_n$) that is exact $\forall f \in \mathcal{P}_{2n+2}$.

Proof

(1) Let $p \in \mathcal{P}_{2n+1}$. This can be written as

$$p \equiv \varphi_{n+1}\, q + r$$

for some $q \in \mathcal{P}_n$ and $r \in \mathcal{P}_n$.

Now

$$I[p] = \int_a^b w(x)\, p(x)\, dx = \int_a^b w(x)\, \varphi_{n+1}(x)\, q(x)\, dx + \int_a^b w(x)\, r(x)\, dx$$

$$\overset{\text{as } \varphi_{n+1} \perp q}{=} \int_a^b w(x)\, r(x)\, dx = I[r].$$

Furthermore,

$$G_n[p] = \sum_{j=0}^{n} w_j\, p(x_j) = \sum_{j=0}^{n} w_j\, \varphi_{n+1}(x_j)\, q(x_j) + \sum_{j=0}^{n} w_j\, r(x_j)$$

$$\overset{\text{as } \varphi_{n+1}(x_j) = 0\ j=0,\ldots,n}{=} \sum_{j=0}^{n} w_j\, r(x_j) = G_n(r)$$

The result follows from $I[r] = G_n(r)$ as for $r \in \mathcal{P}_n$ its Lagrange polynomial of degree n is r.

(2) Let $Q_n[f]$ be any quadrature formula with quadrature points $x_0, x_1, \dots, x_n$.

Let $p(x) = \prod_{j=0}^{n} (x - x_j)^2 \in \mathcal{P}_{2n+2}$.

It follows that

$$Q_n[p] = \sum_{j=0}^{n} w_j \, p(x_j) = 0,$$

whereas

$$I[p] = \int_a^b w(x) \prod_{j=0}^{n} (x - x_j)^2 \, dx$$

$$> 0$$

proving the result. $\square$

Ex

$$I[f] = \int_{-1}^{1} \frac{1}{\sqrt{1-x^2}} f(x) \, dx$$

$$G_1[f] = \pi/2 \, f(-1/\sqrt{2}) + \pi/2 \, f(1/\sqrt{2})$$

$$I[f] = G_1[f] \qquad \forall f \in \mathcal{P}_3$$

THM

Suppose $q \in P_{n+1}$ is such that

$$\langle q, r \rangle = 0 \quad \forall r \in P_j$$

for some $j \in \{0, 1, \ldots, n\}$, and $Q_n[f]$ is the quadrature formula obtained by choosing $x_0, x_1, \ldots, x_n$ as the roots of q. Then

$$I[f] = Q_n[f] \quad \forall f \in P_{n+j+1}.$$

Ex

$$I[f] = \int_{-1}^{1} f(x)\,dx$$

Simpson's rule $Q[f] = \frac{1}{3}\{f(-1) + 4f(0) + f(1)\}$

Let $q(x) = (x+1)(x-0)(x-1) = x^3 - x$.

$$\langle q, 1 \rangle = \int_{-1}^{1} x^3 - x\,dx = 0$$

Hence, by thm above,

$$I[f] = Q[f] \quad \forall f \in P_3$$

THM (Positivity of Weights)

Let $x_0, \ldots, x_n$ be the roots of $\mathcal{U}_{n+1}(x)$. Then

$$\int_a^b w(x) L_k(x)\, dx = \int_a^b w(x) L_k(x)^2\, dx$$

for $k = 0, 1, \ldots, n$.

Proof

As $L_k(x)^2 \in \mathcal{P}_{2n}$, we have

$$I[L_k(x)^2] = G_n[L_k(x)^2].$$

Now

$$I[L_k(x)^2] = \int_a^b w(x) L_k(x)^2\, dx$$

whereas

$$G_n[L_k(x)^2] = w_0 L_k(x_0)^2 + \cdots + w_n L_n(x_n)^2$$
$$= w_k L_k(x_k)^2 = w_k = \int_a^b w(x) L_k(x)\, dx$$

hence the result. $\square$

The convergence of Gaussian quadrature presented next follows from the positivity of the weights. ~~The proof is omitted~~.

THM

For every $f \in C[a,b]$, we have

$$\lim_{n \to \infty} G_n[f] = I[f].$$

Proof

By the Weierstrass approximation thm, for any given $\varepsilon_0 > 0$, there exists a polynomial $p \in \mathcal{P}_{N_0}$ s.t.

$$\| f - p \|_\infty \leqslant \varepsilon_0 .$$

Consider

$$I[f] - G_n[f] = \int_a^b w(x) \{ f(x) - p(x) \} \, dx$$

$$+ I[p] - G_n[p]$$

$$+ G_n[p] - G_n[f],$$

where

$$\left| \int_a^b w(x) \{ f(x) - p(x) \} \, dx \right| \leqslant \underbrace{\int_a^b w(x) \, dx}_{W :=} \, \| f(x) - p(x) \|_\infty$$

$$= \varepsilon_0 W ,$$

and

$$|G_n[p] - G_n[f]| = \left| \sum_{k=0}^{n} w_k \{ p(x_k) - f(x_k) \} \right|$$

$$\leqslant \sum_{k=0}^{n} w_k |p(x_k) - f(x_k)| \leqslant W \varepsilon_0 .$$

since $\sum_{k=0}^{n} w_k = \int_a^b w(x) \cdot 1 \, dx = W$

Furthermore, for all n s.t. $2n+1 \geqslant N_0$, (e.g. $n \geqslant \underbrace{\lceil \frac{N_0 - 1}{2} \rceil}_{N :=}$) we have $I[p] = G_n[p]$. For all such n

$$| I[f] - G_n[f] | \leqslant 2 W \varepsilon_0 .$$

Hence, letting $\varepsilon := 2W\varepsilon_0$,

$$| I[f] - G_n[f] | \leqslant \varepsilon \quad \forall n \geqslant N$$

for some N (depending on ε) proving the result. $\square$

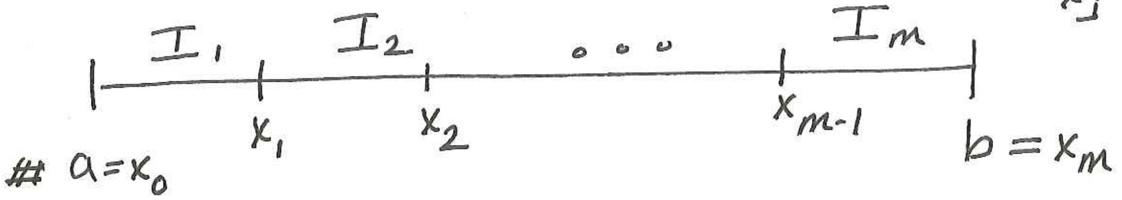
Composite Gaussian Quadrature

Let us focus on

$$I[f] = \int_a^b f(x)\,dx \qquad (\text{i.e. } w(x) \equiv 1)$$

Split $[a,b]$ into m subinterval of equal length $H := (b-a)/m$

$x_j := a + jH$



Apply the same Gaussian quadrature formula on $I_0, I_1, \dots, I_m$.

$$I[f] = \sum_{j=0}^{m-1} \int_{x_j}^{x_{j+1}} f(x)\,dx$$

$[x_j, x_{j+1}]$ can be mapped into $[-1, 1]$ via

$$x = \left(\frac{x_{j+1} - x_j}{2}\right) t + \left(\frac{x_{j+1} + x_j}{2}\right) \quad \left(\begin{array}{l} t=-1 \Leftrightarrow x = x_j \\ t = 1 \Leftrightarrow x = x_{j+1} \end{array}\right.$$

Then

$$(+) \qquad I[f] = \sum_{j=0}^{m-1} \int_{-1}^{1} \underbrace{f\left(\frac{H}{2}t + \frac{H}{2} + x_j\right)}_{g_j(t) :=} \frac{H}{2}\,dt$$

$$= \frac{H}{2} \sum_{j=0}^{m-1} \int_{-1}^{1} g_j(t)\,dt \approx \frac{H}{2} \sum_{j=0}^{m-1} G_n[g_j]$$

Ex

$$I[f] = \int_{-1}^{1} f(x)\,dx$$

Find $G_2[f]$ for $I[f]$ (not the composite one)

$$\varphi_2(x) = \frac{3}{2}x^2 - \frac{1}{2} \quad \left(\text{Legendre polynomial of degree } 2\right)$$

$$x_0 = -1/\sqrt{3} \qquad x_1 = 1/\sqrt{3}$$

$$w_0 = \int_{-1}^{1} \frac{x - 1/\sqrt{3}}{(-2/\sqrt{3})}\,dx = \frac{-\sqrt{3}}{2}\,\frac{(x-1/\sqrt{3})^2}{2}\Bigg|_{-1}^{1} = 1$$

$$w_1 = \int_{-1}^{1} \frac{x + 1/\sqrt{3}}{2/\sqrt{3}}\,dx = 1$$

Hence,

$$G_2[f] = w_0 f(x_0) + w_1 f(x_1)$$
$$= f(-1/\sqrt{3}) + f(1/\sqrt{3})$$

Finding the composite quadrature formula for $I[f] = \int_a^b f(x)\,dx$ with 2-points on each subinterval (Using (+) on page ⑧)

$$I[f] \approx \frac{H}{2} \sum_{j=0}^{m-1} G_2[g_j]$$

$$= \frac{H}{2} \sum_{j=0}^{m-1} \left\{ g_j(-1/\sqrt{3}) + g_j(1/\sqrt{3}) \right\}$$

$$= \frac{H}{2} \sum_{j=0}^{m-1} \left\{ f\left(\left(1-\frac{1}{\sqrt{3}}\right)\frac{H}{2} + x_j\right) + f\left(\left(1+\frac{1}{\sqrt{3}}\right)\frac{H}{2} + x_j\right) \right\}$$