Chapter 5

Numerical integration

In this chapter, we study how to approximate the definite integral of some smooth functions. An idea is to use an interpolating polynomial $F(x)$ to evaluate the integral. Thus we have

$$\int_a^b f(x)\,dx \approx \int_a^b F(x)\,dx.$$

Our purpose is how to design such an interpolation so that the error is minimized.

5.1 Closed Newton-Cotes Formulas

We would like to design a quadrature for the following integral:

$$\int_a^b f(x)\,dx.$$

One point formula: If $F(x)$ is a constant interpolation at x_0, then the above integral is approximated by $(b-a)f(x_0)$ called a **rectangle rule**. One can show that there exist ξ_0 and ξ_0 in $[a,b]$ such that the following hold.

$$\int_a^b f(x)\,dx = \begin{cases} (b-a)f(x_0) + \frac{(b-a)^2}{2} f'(\xi_0), & \text{if } x_0 \neq \frac{b+a}{2} \\ (b-a)f(x_0) + \frac{(b-a)^3}{24} f''(\xi_1), & \text{if } x_0 = \frac{b+a}{2}. \end{cases} \tag{5.1}$$

Thus one point formula is exact for constant polynomial(except mid point rule), so it is called a **0-th order method**.

Two point formula-trapezoidal rule:

$$\int_a^b f(x)\,dx = \frac{b-a}{2}(f(a)+f(b)) - \frac{(b-a)^3}{12} f''(\xi). \tag{5.2}$$

This is exact for linear polynomials, hence it is a **first order method**.

Newton-Cotes Rules

Assume we have nodes $x_0, \cdots, x_n$ in $[a,b]$ are equally spaced. We use an interpolating polynomial $p(x)$ to replace the integral.

$$\int_a^b f(x)\,dx \approx \int_a^b p(x)\,dx = \sum_{i=0}^n c_i p(x_i) = \sum_{i=0}^n c_i f(x_i).$$

For example, if we use the Lagrange interpolating polynomial, we have

$$p_n(x) = \sum_{i=0}^n f(x_i) L_{n,i}(x), \tag{5.3}$$

where

$$L_{n,i}(x) = \prod_{i \neq i}^n \frac{(x-x_j)}{(x_i - x_j)}, \quad 0 \le i \le n.$$

We let

$$\int_a^b f(x)\,dx \sim \sum_{i=0}^n f(x_i) \int_a^b L_{n,i}(x)\,dx = \sum_{i=0}^n B_{n,i} f(x_i),$$

where

$$B_{n,i} = \int_a^b L_{n,i}(x)\,dx.$$

This is the **Newton-Cotes formula**. If $x_0 = a$ and $x_n = b$, then we say it is a **closed Newton-Cotes formula**. Otherwise, it is called an **open Newton-Cotes formula**. Mid point rule is an open Newton-Cotes formula.

Three point formula-Simpson rule

Use an interpolation at three equally spaced points x_0, x_1, x_2 : Let

$$\int_{x_0}^{x_2} f(x)\,dx \approx \int_{x_0}^{x_2} p_2(x)\,dx, \tag{5.4}$$

where $p_2(x)$ is the Lagrange interpolation. For simplicity, we assume $x_0 = -h, x_1 = 0$ and $x_2 = h$. Then

$$p_2 = f(x_0)\frac{x(x-h)}{2h^2} + f(x_1)\frac{(x+h)(x-h)}{-h^2} + f(x_2)\frac{(x+h)x}{2h^2}.$$

Integrating, we obtain

$$\begin{aligned}
&= \int_{-h}^{h} \frac{1}{2h^2}\left[(f_0 - 2f_1 + f_2)x^2 + (-hf_0 + hf_2)x + 2h^2\right] dx \\
&= \frac{1}{2h^2}\left[\frac{h^3}{3}(f_0 - 2f_1 + f_2) + 4h^3 f_1\right] \\
&= \frac{h}{3}(f_0 + 4f_1 + f_2).
\end{aligned}$$

Hence we get the following rule, called the **Simpson's rule**

$$\int_{x_0}^{x_2} f(x)\,dx \sim \frac{h}{3}(f(x_0) + 4f(x_1) + f(x_2)) \equiv s_1(f). \tag{5.5}$$

One can readily check that this is exact for a polynomial up to degree three, even if we used a quadratic polynomial approximation. Hence this is a third order method. In fact one can show that

$$\int_{x_0}^{x_2} f(x)\,dx = \frac{h}{3}(f(x_0) + 4f(x_1) + f(x_2)) - \frac{h^5}{90}f^{(4)}(\xi_1), \quad \xi_1 \in [x_0, x_2]. \tag{5.6}$$

Similar phenomenon arises for all even n. Derive formula for $n = 3$ and $n = 4$.

Error of numerical integration

We consider **Newton-Cotes formula**. We assume the following situation: Let $a \le x_0 < x_1 < \cdots < x_n \le b$, $x_i - x_{i-1} = h$ and consider an approximation of $\int_a^b f(x)dx$ by some quadrature based on the data $(x_0, f(x_0), \cdots, (x_n, f(x_n))$. Use Taylor formula with remainder:

$$f(x) = f(x_0) + f'(x_0)(x-x_0) + \cdots + \frac{f^{(n)}(x_0)}{n!}(x-x_0)^n + \frac{f^{(n+1)}(\xi)}{(n+1)!}(x-x_0)^{n+1}$$

or Newton's interpolating polynomial

$$p_n(f) = f(x_0) + f[x_0, x_1](x-x_0) + \cdots + f[x_0, x_1, \cdots, x_n](x-x_0)\cdots(x-x_{n-1}).$$

By the error formula, we have

$$f(x) = p_n(f) + f[x_0, x_1, \cdots, x_n, x](x - x_0) \cdots (x - x_n).$$

Integrating the error term of Newton's formula we have

$$E(f) = \int_a^b f[x_0, x_1, \cdots, x_n, x] \prod_{i=0}^{n} (x - x_i) dx = \int_a^b \frac{f^{(n+1)}(\xi)}{(n+1)!} \prod_{i=0}^{n} (x - x_i) dx.$$

Since the term $\prod_{i=0}^{n}(x-x_i)$ does not change sign on each subinterval (x_s, x_{s+1}), we can use mean value theorem to see the above quantity is

$$\frac{f^{(n+1)}(\bar{\xi}_s)}{(n+1)!} \int_{x_s}^{x_{s+1}} \prod_{i=0}^{n} (x - x_i) dx = \frac{f^{(n+1)}(\bar{\xi}_s)}{(n+1)!} \times O(h^{n+2}),$$

for some $\bar{\xi}_s \in (x_s, x_{s+1})$. A more precise error formula is as follows:(See Issacson-Keller)

Theorem 5.1.1. *The error by Newton-Cotes formula is*

$$E(f) = \begin{cases} \dfrac{f^{(n+2)}(\bar{\xi})}{(n+2)!} \displaystyle\int_a^b (x - x_0) \prod_{i=0}^{n} (x - x_i) dx, & \text{if } n \text{ is even} \\ \dfrac{f^{(n+1)}(\bar{\xi})}{(n+1)!} \displaystyle\int_a^b \prod_{i=0}^{n} (x - x_i) dx, & \text{if } n \text{ is odd.} \end{cases} \tag{5.7}$$

As noted earlier, we have one higher order of accuracy for even n.

Semi-Simpson rule

If n is odd, we can approximate

$$\int_{x_0}^{x_{n-1}} f(x)\, dx$$

by Simpson's rule, but to apply Simpson's rule to

$$\int_{x_0}^{x_n} f(x)\, dx$$

we split the integral into two parts:

$$\int_{x_0}^{x_n} f(x)\, dx = \int_{x_0}^{x_{n-1}} f(x)\, dx + \int_{x_{n-1}}^{x_n} f(x)\, dx$$

and we can apply Simpson's rule to the first integral. But how to approximate the second integral (we need the same order method)?

One idea is to add an extra point, say x_{n-2} and use a quadratic interpolation:

$$p_2(x) = f_{n-2}\frac{(x-x_{n-1})(x-x_n)}{(-h)(-2h)} + f_{n-1}\frac{(x-x_{n-2})(x-x_n)}{(h)(-h)} + f_n\frac{(x-x_{n-2})(x-x_{n-1})}{(2h)(h)}.$$

Change of variable: $x - x_{n-1} = th$ gives

$$p_2(x) = f_{n-2}\frac{(t-1)(t-2)}{2} - f_{n-1}t(t-2) + f_n\frac{t(t-1)}{2}.$$

Thus

$$\begin{aligned}\int_{x_{n-1}}^{x_n} f(x)\,dx &\approx h\int_1^2 f_{n-2}\frac{(t-1)(t-2)}{2} - f_{n-1}t(t-2) + f_n\frac{t(t-1)}{2}\,dt\\ &= \frac{h}{12}(-f(x_{n-2}) + 8f(x_{n-1}) + 5f(x_n)).\end{aligned}$$

Ex. Derive an integration rule for $\int_{x_0}^{x_1} f(x)\,dx$ using the data at x_0, x_1 and x_2(assume $h = x_1 - x_0 = x_2 - x_1$.)

Composite Simpson's rule

If the domain is large, divide it by even number of intervals and applying Simpson's rule to a pair of subintervals, one can find a more accurate approximation. Let $x_i = a + ih, h = (b-a)/2n$. Then

$$\int_a^b f(x)\,dx = \int_{x_0}^{x_2} f(x)\,dx + \int_{x_2}^{x_4} f(x)\,dx + \cdots + \int_{x_{2n-2}}^{x_{2n}} f(x)\,dx.$$

If Simpson's rule is used for each integral, we obtain

$$\int_a^b f(x)\,dx \sim \frac{h}{3}\sum_{i=1}^{n}[f(x_{2i-2}) + 4f(x_{2i-1}) + f(x_{2i})].$$

To avoid repetitions it is rearranged as

$$\frac{h}{3}\left[f(x_0) + 2\sum_{i=2}^{n} f(x_{2i-2}) + 4\sum_{i=1}^{n} f(x_{2i-1}) + f(x_{2n})\right].$$

5.2 Open Newton-Cotes Formulas

We consider approximation of integral $\int_a^b f(x)dx$ by interpolating at $n+1$ *interior points*

$$x_0 = a+h, x_1 = a+2h, \cdots, x_n = a+(n+1)h.$$

Here $h = (b-a)/(n+2)$.This rule is useful when we cannot use or do not want to use end points.

(1) $n = 0$: $\int_a^b f(x)dx \approx 2hf(x_0)$. Error: $\frac{h^3}{3}f''(\xi)$

(2) $n = 1$: $\int_a^b f(x)dx \approx \frac{3h}{2}(f(x_0)+f(x_1))$. Error: $\frac{3h^3}{4}f''(\xi)$

(3) $n = 2$: $\int_a^b f(x)dx \approx \frac{4h}{3}(2f(x_0)-f(x_1)+2f(x_2))$. Error: $\frac{14h^5}{45}f^{(4)}(\xi)$

Notice that even cases are more accurate.

How to find the coefficients? One way is to integrate the Lagrange interpolation

$$\int_a^b f(x)\,dx \sim \sum_{i=0}^n w_i f(x_i), \tag{5.8}$$

where

$$w_i = \int_a^b L_{n,i}(x)\,dx.$$

Another method is to let the formula (5.8) be exact for all monomials x^i, $(i = 0, 1, \cdots, n.)$ For $n = 3$

$$\int_a^b f(x)\,dx \sim \frac{5h}{24}\left(11f(x_0)+f(x_1)+f(x_2)+11f(x_3)\right) \tag{5.9}$$

Remark 5.2.1. In general, open Cotes rules are used much less than the closed rule. However, there are instances where end points not available.

5.3 Gaussian quadrature-unequal intervals

We now consider a quadrature with unequal intervals. Check that the quadrature

$$\int_{-1}^1 f(x)\,dx \doteq f(-\sqrt{\frac{1}{3}})+f(\sqrt{\frac{1}{3}})$$

is exact up to degree 3. The degree of precision of the following quadrature is 5.

$$\int_{-1}^{1} f(x)\,dx \doteq \frac{5}{9}f(-\sqrt{\frac{3}{5}}) + \frac{8}{9}f(0) + \frac{5}{9}f(\sqrt{\frac{3}{5}}).$$

General three point formula with weight is of the form:

$$\alpha_0 f(\beta_0) + \alpha_1 f(\beta_1) + \alpha_2 f(\beta_2).$$

More generally, we consider

$$\int_a^b f(x)w(x)dx \approx \sum_{i=0}^{n} A_i f(x_i), \tag{5.10}$$

where w is a fixed *positive* weight function. Here we have freedom of choice of x_i as well as the coefficients. This weight may be useful if we need to evaluate an integral of functions of the form $g(x) = f(x)w(x)$.

This formula is exact for polynomial of degree up to n if and only if(let $f(x) = L_{n,i}(x)$)

$$A_i = \int_a^b w(x) \prod_{j \neq i}^{n} \frac{x - x_j}{x_i - x_j} dx.$$

Note that there are no restrictions on the nodes. By placing nodes at proper places, we can obtain $2n + 1$ order of approximation.

Example 5.3.1. Let $w(x) = (1 - x^2)^{-1/2}$. Then

$$\int_{-1}^{1} \frac{f(x)}{(1 - x^2)^{1/2}}\, dx \approx \frac{\pi}{n+1} \sum_{k=0}^{n} f(x_k)$$

with $x_k = \cos(\frac{(k+1/2)\pi}{n+1}),\ k = 0, \cdots, n$ is exact for a polynomial degree up to $2n + 1$.

Example 5.3.2. With $n = 1$ on $[-1, 1]$, $x_0 = \cos(\pi/4) = 1/\sqrt{2}$ and $x_1 = \cos(3\pi/4) = -1/\sqrt{2}$. So

$$\begin{aligned}
\int_{-1}^{1} \frac{x^2}{(1 - x^2)^{1/2}}\, dx &\approx \frac{\pi}{2}(f(x_0) + f(x_1)) \\
&= \frac{\pi}{2}(\frac{1}{2} + \frac{1}{2}) \\
&= \frac{\pi}{2}.
\end{aligned}$$

It can be shown that this is exact.

Inner Product Space

We define the inner product of functions w.r.t a (positive) weight function $w(x)$ over an interval $[a, b]$. Given $f, g \in V(V$ is a vector space of functions defined over $[a, b])$, let

$$(f, g) = \int_a^b f(x)g(x)w(x)\,dx. \tag{5.11}$$

It can easily be shown that it satisfies usual properties of inner product:

(1) $(f, f) \geq 0$ for all f and $(f, f) = 0$ only if $f = 0$.

(2) $(f, g) = (g, f)$

(3) $(\alpha f + \beta f, h) = \alpha(f, h) + \beta(g, h)$ for scalar α, β.

If $V = P_n$ the set of all polynomials degree less than equal to n. The obvious basis for V is $\{1, x, x^2, \cdots, x^n\}$. But we would like to have an *orthogonal basis.* Thus we use Gram-Schmidt process. Let $w(x) = 1$, $[a, b] = [-1, 1]$ and

$$m_0 = 1, m_1 = x, m_2 = x^2, \cdots, m_n = x^n.$$

We find $p_0 = 1$ and

$$\begin{aligned} p_1(x) &= m_1 - \frac{(p_0, m_1)}{(p_0, p_0)} p_0(x) \\ &= x - \frac{1}{2}(\int_{-1}^{1} 1 \cdot x w(x)\,dx) \cdot 1 \\ &= x \end{aligned}$$

$$\begin{aligned} p_2(x) &= m_2 - \frac{(p_0, m_2)}{(p_0, p_0)} p_0(x) - \frac{(p_1, m_2)}{(p_1, p_1)} p_1(x) \\ &= x^2 - \frac{1}{2}(\int_{-1}^{1} 1 \cdot x^2\,dx) \cdot 1 - \frac{1}{(p_1, p_1)}(\int_{-1}^{1} p_1 \cdot x^2\,dx) \cdot p_1(x) \\ &= x^2 - \frac{1}{3} \end{aligned}$$

Note these are not normalized.

Theorem 5.3.3. *Let q be a nonzero polynomial of degree $n+1$ which is orthogonal to P_n(the set of all polynomials of degree $\leq n$) with respect to the weight w, i.e, we have*

$$\int_a^b q(x)p(x)w(x)dx = 0, \text{ for all } p(x) \in P_n.$$

If $x_0, x_1, \cdots, x_n$ are the zeros of q, then the quadrature formula (5.10) is exact for all $f \in P_{2n+1}$.

Proof. Let $f \in P_{2n+1}$. Dividing f by q, we obtain the quotient p and remainder r. Hence

$$f = qp + r \quad (\text{degree of } p \text{ and } , r < n+1)$$

and $f(x_i) = r(x_i)$. Since q is orthogonal to p with respect to w and the formula (5.10) is exact for polynomial of degree n, we have

$$\int_a^b fw\,dx = \int_a^b rw\,dx = \sum_{i=0}^n A_i r(x_i) = \sum_{i=0}^n A_i f(x_i).$$

□

Now the remaining task is to find orthogonal polynomials and their zeros. Fortunately, some cases are well-known: Let $[-1,1]$. Then with $w = 1$, the Legendre polynomials are ortho-normal polynomials on $[-1,1]$. i.e,

$$\int_{-1}^1 p_n(x)p_m(x)\,dx = \delta_{nm}.$$

$$\begin{aligned}
p_0(x) &= \frac{1}{\sqrt{2}}, \quad p_1(x) = \sqrt{\frac{3}{2}}x \\
p_2(x) &= \sqrt{\frac{5}{2}}\frac{1}{2}(3x^2-1), \quad p_3(x) = \sqrt{\frac{7}{2}}\frac{1}{2}(5x^3-3x) \\
p_4(x) &= \sqrt{\frac{9}{2}}\frac{1}{8}(35x^4-30x^2+3), \quad p_5(x) = \sqrt{\frac{11}{2}}\frac{1}{8}(63x^5-70x^3+15x) \\
p_6(x) &= \sqrt{\frac{13}{2}}\frac{1}{24}(7\cdot 33x^6 - 63\cdot 5x^4 + 35\cdot 3x^2 - 5) \\
&\ \ ,\cdots, \\
p_n(x) &= \left(n+\frac{1}{2}\right)^{1/2}\frac{1}{n!\,2^n}\frac{d^n}{dx^n}(x^2-1)^n.
\end{aligned}$$

Exercise 5.3.4. Let

$$\Phi_n(x) = \frac{1}{n!\,2^n}\frac{d^n}{dx^n}(x^2-1)^n$$

Then

(1) $\Phi_n(1) = 1$, $\Phi_n(-1) = (-1)^n$

(2) Φ_n is generated by the recursive formula

$$\Phi_{n+1} = \frac{2n+1}{n+1}x\Phi_n - \frac{n}{n+1}\Phi_{n-1},\ \ \Phi_0 = 1,\ \ \Phi_1 = x$$

(3) $\Phi_n(x)$ is a solution of Legendre differential equation

$$(1-x^2)y'' - 2xy' + n(n+1)y = 0.$$

5.3.1 Error of Gaussian quadrature

Lemma 5.3.5. *In Gaussian quadrature, the coefficients are positive and their sum is* $\int_a^b w(x)dx$. *In particular, if* $[a,b] = [-1,1]$ *and* $w \equiv 1$, *then* $\sum_{i=0}^n A_i = 2$.

Proof. Fix n and let q be a polynomial of degree $n+1$ which is orthogonal to P_n. The zeros of q are denoted by $x_0,\cdots,x_n$. Let $p(x) = q(x)/(x-x_j)$ for some j. Since p^2 is of degree at most $2n$, Gaussian quadrature with $x_0,\cdots,x_n$ will be exact for p^2. Hence

$$0 < \int_a^b p^2(x)w(x)dx = \sum_{i=0}^n A_i p^2(x_i) = A_j p^2(x_j)$$

so that $A_j > 0$. Now use Gaussian quadrature for $f(x) = 1$ to see

$$\int_a^b w(x)dx = \sum_{i=0}^n A_i.$$

□

Theorem 5.3.6. *For any* $f \in C^{2n+2}[a,b]$, *the error term* E *in the Gaussian quadrature*

$$\int_a^b f(x)w(x)dx = \sum_{i=0}^n A_i f(x_i) + E$$

satisfies

$$E = \frac{f^{(2n+2)}(\xi)}{(2n+2)!} \int_a^b q^2(x) w(x) dx$$

for some $a < \bar{\xi} < b$ *and* $q(x) = \prod_{i=0}^{n} (x - x_i)$.

References

(1) Philip J. Davis and P. Rabinowitz. Methods of Numerical Integration, 2nd ed, 1984. AP.

(2) Philip J. Davis, Interpolation and Approximation, 1963 Dover

(3) Hildebrand, F.B. Introduction to Numerical analysis, 1956, McGraw-Hill.

(4) Carl-Erik Froberg, Numerical mathematics, 1985 Benjamin/Cummings Pub. Company inc. pp. 288–296.

(5) http:/mathworld.wolfram.com/Chebyshev-GaussQuadrature.html

(6) http:/mathworld.wolfram.com/LobattoQuadrature.html

(7) http:/mathworld.wolfram.com/RadauQuadrature.html

(8) Handbook of Mathematical Functions with Formulas, Graphs and Mathematical Tables, Abramowitz, M. and Stegun

5.4 More on Gauss type quadrature

We now consider the case $w(x) \neq 1$. One example is $w(x) = exp(-x)$(Gauss-Laguerre) which is useful in $\int_0^\infty f(x) exp(-x) dx$.

Let $\Phi_i(x)$ for $i = 0, \cdots, n$ be orthonormal polynomials w.r.t weight $w(x)$. Observe

$$\Phi_{n+1}(x) - ax\Phi_n(x) = \sum_{i=0}^{n} \alpha_i \Phi_i(x) \tag{5.12}$$

for some scalar a and α_i. HW. Determine a and α_i using the orthogonality. Show that $\alpha_i = 0$ for $i = n-2, n-3, \cdots, 0$.

General Gauss Chebysheff quadrature

If we use $w(x) = \frac{1}{\sqrt{1-x^2}}$ the corresponding orthogonal polynomials are the Chebysheff polynomial of first kind and using these, we obtain the Gauss Chebysheff quadrature. The nodes x_i are the zeros of orthogonal polynomial w.r.t. $w(x) = \frac{1}{\sqrt{1-x^2}}$.

It is known that the Chebysheff polynomial satisfies

$$\int_{-1}^{1} T_m(x)T_n(x)\frac{1}{\sqrt{1-x^2}}\,dx = c_{mn}\delta_{mn}$$

and hence the interpolating points are the Chebysheff points:

$$x_k = \cos\left(\frac{2k+1}{2(n+1)}\pi\right), \quad k = 0, \cdots, n$$

Thus Gauss Chebysheff quadrature with weight $w(x) = \frac{1}{\sqrt{1-x^2}}$ based on $n+1$ points for $[-1, 1]$ is

$$\int_{-1}^{1} f(x)w(x)\,dx = \sum_{i=0}^{n} A_i f(x_i),$$

where $x_i, i = 0, \cdots, n$ are the zeros of $T_{n+1}(x)$ and it can be shown that

$$A_i = \int_{-1}^{1} \frac{L_{n,i}(x)}{\sqrt{1-x^2}}\,dx = \frac{\pi}{n+1}, \quad i = 0, \cdots, n$$

Remark 5.4.1. The first two Chebysheff polynomials are $T_0(x) = 1$, $T_1(x) = x$ and in general

$$T_n(x) = \frac{1}{2^{n-1}}\cos(n\cos^{-1}(x)) \tag{5.13}$$

and hence

$$x_k = \cos\left(\frac{2k+1}{2n}\pi\right).$$

Notice the points are densely packed near the boundary; thus it may be good for function which is unbounded near the boundary. Find the coefficients in

$$T_{n+1}(x) = axT_n(x) + \alpha T_{n-1}(x) \tag{5.14}$$

for $n \geq 2$. If we use $w(x) = \sqrt{1-x^2}$ instead, we obtain Chebysheff polynomial of second kind and hence obtain Gauss Chebysheff quadrature of second kind which will not be discussed further.

Theorem 5.4.2. *If $q(x)$ is a monic polynomial of degree n then*

$$\max_{[-1,1]} |T_n(x)| = \frac{1}{2^{n-1}} \leq \max_{[-1,1]} |q(x)|.$$

Thus $T_n(x)$ has the 'smallest' size(measured in maximum norm) among all polynomial of degree n. Stated another way, its deviation from 0 is smallest.

Proof. Suppose there is a monic poly. $p(x)$ such that

$$|p(x)| < 2^{1-n}, \ |x| \leq 1.$$

Let $y_i = \cos(i\pi/n), 0 \leq i \leq n$. Then $T_n(y_i) = (-1)^i 2^{1-n}$. Since T_n is a monic poly. of degree n

$$(-1)^i p(y_i) \leq |p(y_i)| < 2^{1-n} = (-1)^i T_n(y_i).$$

Hence

$$(-1)^i (T_n(y_i) - p(y_i)) > 0 \ (0 \leq i \leq n).$$

This means the polynomial $T_n(x) - p(x)$ oscillates $n+1$ times in sign and hence must have at least n roots in $(-1, 1)$. This is impossible since $T_n(x) - p(x)$ is degree $n - 1$. □

Recall

$$f(x) - p_n(x) = \frac{f^{(n+1)}(\xi(x))}{(n+1)!} \prod_{i=0}^{n} (x - x_i). \tag{5.15}$$

We cannot control the coefficient term. However, we can control

$$\omega(x) = (x - x_0)(x - x_1) \cdots (x - x_n).$$

This is minmized over $[-1, 1]$ by choosing the nodes the $n + 1$ Chebysheff points.

The use of Chebysheff points gives the interpolating polynomial that minimizes the maximum $|f(x) - p(x)|$ ($\|f - p\|_\infty$). It can be shown that

$$w_i = \int_{-1}^{1} \frac{L_i(x)}{\sqrt{1 - x^2}} \, dx = \frac{\pi}{n + 1}, \quad i = 0, \cdots, n$$

Proof. Observe that for all $k = 0, 1, \cdots, n$

$$(x - x_k)L_k(x) = c_k p_{n+1}(x)$$

Thus

$$\begin{aligned} w_i &= \int_{-1}^{1} L_i(x)\,dx \\ &= \int_{-1}^{1} \frac{c_i p_{n+1}(x)}{(x - x_i)}\,dx \end{aligned}$$

□

Example 5.4.3. Use G-Chebysheff quadrature $n = 4$ to approximate $\int_{-1}^{1} \cos(\pi x)\,dx$.

$$\begin{aligned} \int_{-1}^{1} \cos(\pi x)\,dx &= \int_{-1}^{1} \cos(\pi x)\sqrt{1 - x^2}\frac{1}{\sqrt{1 - x^2}}\,dx \\ &= \int_{-1}^{1} f(x)w(x)\,dx \\ &= \frac{\pi}{5}\left[f(\cos(\frac{\pi}{10})) + f(\cos(\frac{3\pi}{10})) + f(\cos(\frac{5\pi}{10})) + f(\cos(\frac{7\pi}{10})) + \cdots \right] \end{aligned}$$

It is always possible to generate orthogonal polynomials by

$$p_{n+1}(x) = x p_n(x) - \alpha_{n+1} p_n(x) - \beta_{n+1} p_{n-1}(x), \tag{5.16}$$

where

$$\begin{aligned} \alpha_{n+1} &= \frac{(p_n, x p_n)}{(p_n, p_n)} \\ \beta_{n+1} &= \frac{(p_n, x p_{n-1})}{(p_{n-1}, p_{n-1})} \end{aligned}$$

and $p_{-1}(x) = 0$.

Gauss Lobatto quadrature

Let ϕ_n be the Legendre polynomial of degree n on $[-1, 1]$ and let $x_i, i = 0, \cdots, n$ be the zeros of $p = \phi_{n+1}(x) + \lambda\phi_n(x) + \mu\phi_{n-1}(x)$. Here λ, μ are chosen so that $p(-1) = p(1) = 0$. Then we have $x_0 = -1$ and $x_n = 1$. Now consider the following quadrature

$$A_0 f(x_0) + A_n f(x_n) + \sum_{i=1}^{n-1} A_i f(x_i) \tag{5.17}$$

to approximate $\int_{-1}^{1} f(x)dx$. Here we A_i's are determined by letting the above quadrature is exact for $f = 1, x, \cdots, x^n$.

Theorem 5.4.4. *The quadrature (5.17) is exact for polynomials degree up to* $2n-1$.

Proof. First λ, μ are determined by $p(-1) = p(1) = 0$. Assume the formula is exact for P_n. Let f be in P_{2n-1}. Then dividing f by p, we can write $f = pq + r$ for some $q \in P_{n-2}$ and $r \in P_n$.

$$\begin{aligned}
\int_{-1}^{1} f(x)dx &= \int_{-1}^{1} pq\,dx + \int_{-1}^{1} r\,dx \\
&= 0 + \int_{-1}^{1} r\,dx (\text{ orthogonality }) \\
&= \sum_{i=0}^{n} A_i r(x_i) (\text{ since } r \text{ is degree } n\text{ }) \\
&= \sum_{i=0}^{n} A_i f(x_i) (\text{ since } p(x_i) = 0 \text{ for } i = 0, \cdots, n).
\end{aligned}$$

□

Some difficulty may arise if one tries to find the interpolation points x_i.

Example 5.4.5. For $n = 3$, we first note that

$$p = 35x^4 - 30x^2 + 3 + \lambda(5x^3 - 3x) + \mu(3x^2 - 1).$$

Using $p(\pm 1) = 0$, we get $\lambda = 0, \mu = -4$. Hence

$$p(x) = 35x^4 - 42x^2 + 7 = 7(5x^2 - 1)(x^2 - 1).$$

Thus $x_1 = -\frac{1}{\sqrt{5}}$, $x_2 = \frac{1}{\sqrt{5}}$.

When $n = 3$, there is a special method to find the formula. Assume the following symmetric formula:

$$A_0 f(-1) + A_1 f(-x_1) + A_1 f(x_1) + A_0 f(1).$$

By symmetry, it is exact for any odd degree polynomial. We can find A_0, A_1 and x_1 by imposing the condition that it is exact for $f = 1, x^2, x^4$.

$$\begin{aligned} A_0 + A_1 &= 1 \\ A_0 + A_1 x_1^2 &= \frac{1}{3} \\ A_0 + A_1 x_1^4 &= \frac{1}{5}. \end{aligned}$$

Solving we get $x_1 = -\frac{1}{\sqrt{5}}$. Thus, the Gauss-Lobatto formula in this case is

$$\frac{1}{6}f(-1) + \frac{5}{6}f(-\frac{1}{\sqrt{5}}) + \frac{5}{6}f(\frac{1}{\sqrt{5}}) + \frac{1}{6}f(1).$$

(For other general formula, See p355 Num. anal. by Jeffery Leader, Addison Wesley or Beurling's book.)

Assume the formula

$$A_0 f(-1) + A_n f(-x_1) + \sum_{i=1}^{n} A_i f(x_i)$$

is exact up to degree $2n-1$. where the sum is up to $n/2$ for n even and up to $(n+1)/2$ for n odd.

$$\begin{aligned} f = 1: &\qquad A_0 + A_n + \sum_{i=1}^{n-1} A_i = 2 \\ f = x: &\qquad -A_0 + A_n + \sum_{i=1}^{n-1} A_i x_i = 0 \\ : &\qquad \cdots \\ f = x^k: &\qquad A_0 + A_n + \sum_{i=1}^{n-1} A_i x_i^k = \frac{2}{k+1} \\ &\qquad \cdots \\ f = x^n: &\qquad A_0 + A_n + \sum_{i=1}^{n-1} A_i x_i^n = \frac{2}{n+1} \end{aligned}$$

for even k.

Weight and points of Gauss Lobatto quadrature

Let $\Phi_n(x)$ be the unnormalized Legendre polynomial of degree n and let $\phi_n(x)$ be its normalized(leading coefficient is 1) Legendre polynomial. Let $k_n = \frac{(2n)!}{2^n(n!)^2}$ be the leading coefficients of $\Phi_n(x)$. Then general Gauss Lobatto quadrature based on $n+1$ points for $[-1,1]$ is

$$\int_{-1}^{1} f(x)dx = \frac{2}{n(n+1)}(f(-1)+f(1)) + \sum_{i=1}^{n-1} A_i f(x_i),$$

where $x_i, i = 1, \cdots, n-1$ are zeros of $\phi_n'(x)$, the derivative of Legendre polynomial of degree n and

$$A_i = \frac{2}{n(n+1)k_n^2\phi_n^2(x_i)}$$

The error is of the form

$$E = c_n f^{(2n)}(\xi)$$

which is exact up to degree $2n-1$ compared to the $2n+1$(Gauss quadrature); we have given up the freedom of location of points.

General Gauss Radau quadrature

Let $\Phi_n(x)$ be the unnormalized Legendre polynomial of degree n and let $\phi_n(x)$ be its normalized(leading coefficient is 1) Legendre polynomial. Let $k_n = \frac{(2n)!}{2^n(n!)^2}$ be the leading coefficients of $\Phi_n(x)$. Then the general Gauss Radau quadrature based on $n+1$ points(the point -1 plus n points in the open interval) for $[-1,1]$ is

$$\int_{-1}^{1} f(x)dx = \frac{2}{(n+1)^2} f(-1) + \sum_{i=1}^{n} A_i f(x_i)$$

where $x_i, i = 1, \cdots, n$ are the zeros of

$$\frac{k_n\phi_n(x) + k_{n+1}\phi_{n+1}(x)}{x-1}$$

and

$$A_i = \frac{1-x_i}{(n+1)^2 k_n^2 \phi_n^2(x_i)}, i = 1, \cdots, n$$

The error is of the form

$$E = d_n f^{(2n+1)}(\xi).$$