Introduction to Numerical Analysis I
Handout 11

1 Numerical Differentiation and Integration (cont)

1.2 Numerical Integration (cont)

1.2.1 Integration using Interpolation (cont)

Composite Rules All the priorly discussed quadratures implicitly considered $h \to 0$. We consider now a big interval $[a, b]$ divided into subintervals for integration.

Composite Trapezoidal Rule Consider a uniform grid $x_j = a + jh$ where $j = 0, \ldots, n$ and $h = \frac{b-a}{n}$ then

$$\int_a^b f(x)\,dx = \sum_{j=0}^{n} \int_{x_j}^{x_j+h=x_{j+1}} f(x)\,dx =$$

$$\sum_{j=0}^{n} \left\{ h\frac{f(x_j)+f(x_{j+1})}{2} + O\left(h^3\right) \right\} =$$

$$= \underbrace{\frac{b-a}{n}}_{h} \left(\frac{f(a)}{2} + \sum_{k=1}^{n-1} f(x_j) + \frac{f(b)}{2} \right) - \underbrace{n \cdot \frac{f''(c)}{12} h^3}_{O\left(h^2\right)}$$

Note: The formula of the quadrature remains the same for any set $a = x_0 \leq \ldots \leq x_n = b$.

Composite Simpson Rule Similarly, for the grid $x_k = a + kh,\ \ h = \frac{b-a}{2n},\ \ k = 0, \ldots, 2n$ one gets

$$\int_a^b f(x)\,dx = \sum_{j=0}^{n-1} \frac{h}{3} \left\{ f(x_{2n}) + 4f(x_{2n+1}) + f(x_{2n+2}) + O\left(h^5\right) \right\}$$

$$= \frac{h}{3} \left\{ f(a) + 2\sum_{j=1}^{n-1} f(x_{2n}) + 4\sum_{j=0}^{n-1} f(x_{2n+1}) + f(b) + nO\left(h^5\right) \right\}$$

$$= \frac{h}{3} \left\{ f(a) + 4f(x_1) + 2f(x_2) + 4f(x_3) + \ldots + f(b) \right\}$$

$$-\frac{b-a}{2h}\frac{h^5}{90} \max_{x\in[a,b]} \left\{ \left| f^{(4)}(x) \right| \right\}$$

Example 1.1. How many points required to approximate $\int_0^\pi \sin x\,dx$ with error bounded by 10^{-2} using composite Trapezoidal method.

Since $\max\limits_{x\in[0,\pi]} \left|\sin^{(2)} x\right| = 1$ one gets

$$\left|\frac{f''(\xi)}{12}\pi h^2\right| \leqslant \frac{\pi}{12}h^2 \leqslant 10^{-2}, \text{ that is}$$

$\frac{\pi}{n} = h \leqslant \sqrt{\frac{12}{\pi}10^{-2}} \approx \sqrt{0.038} \leqslant 0.2$, thus $n \geqslant 16$.

1.2.2 Integration using polynomial basis

One develops quadratures using Algebraic Order of Exactness (similar to what we did with differentiation)

Trapezoidal Rule Consider a quadrature of the following form $\int_a^b f(x)\,dx \approx A_0 f(a) + A_1 f(b)$, exact for the $f = 1$ and $f = x$. The linear system is

$$\begin{cases} \int_a^b 1dx = b - a & = A_0 + A_1 \\ \int_a^b xdx = \frac{b^2 - a^2}{2} & = aA_0 + bA_1 \end{cases}$$

and the solution is $A_0 = A_1 = \frac{b-a}{2}$, which gives the trapezoidal rule, and shows it has the algebraic exactness of 1.

Simpson Rule Similarly consider quadrature of the form of $\int_a^b f(x)\,dx \approx A_0 f(a) + A_1 f\left(\frac{a+b}{2}\right) + A_2 f(b)$ exact for $1, x$ and x^2. The linear system become

$$\begin{cases} \int_a^b 1dx = b - a & = A_0 + A_1 + A_2 \\ \int_a^b xdx = \frac{b^2 - a^2}{2} & = aA_0 + \frac{a+b}{2}A_1 + bA_2 \\ \int_a^b x^2dx = \frac{b^3 - a^3}{3} & = a^2A_0 + \frac{(a+b)^2}{4}A_1 + b^2A_2 \end{cases}$$

which has a solution $(A_0, A_1, A_2) = \frac{b-a}{6}(1, 4, 1)$, which gives the Simpson's rule and shows it has the algebraic exactness of 2.

1.2.3 Gaussian quadrature

We now developing quadratures for $\int_a^b w(x) f(x)\,dx$ where $w(x)$ denotes weight function.

Orthogonal Polynomials

Definition 1.2 (**Vector Space (briefly)**)**.** A vector space V over a (scalar) field F is a set that is closed under finite vector addition ($u, v \in V \Rightarrow u + v \in V$) and scalar multiplication ($c \in F, u \in V \Rightarrow cu \in V$).

Definition 1.3 (**Inner Product**)**.** Let V be a subspace of a vector space over a field of complex numbers $F \subset C$. Let $u, v \in V$. The function $(u, v) : V \times V \mapsto C$ is called inner product if the following holds:

1. $(u, u) \geq 0$ and $(u, u) = 0$ iff $u = 0$.
2. $(u, v) = \overline{(v, u)}$ where $\bar{u}$ is the complex conjugate of u; for V over reals $(u, v) = (v, u)$.
3. $(u_1 + u_2, v) = (u_1, v) + (u_2, v)$ for $u_1, u_2, v \in V$.
4. $c(u, v) = (cu, v) = (u, \bar{c}v))$ for any scalar $c \in F$.

We concentrate in the V of continuous functions on an interval $[a,b]$ over reals and the inner product with the weight function $w(x) \geq 0$ as following:

$$(f,g) = \int_a^b f(x)\overline{g(x)}w(x)dx \underset{F \subset R}{=} \int_a^b f(x)g(x)w(x)dx$$

Definition 1.4 (**Orthogonality).** We say that the functions (vectors) f and g are orthogonal iff $(f,g) = 0$.

Theorem 1.5 (**The Gram-Schmidt Process).** Let $\{b_j\}_{j=0}^n$ be some basis for a vector space V. The orthogonal basis $\{v_j\}_{j=0}^n$ is defined by

$v_0 = b_0, \qquad v_k = b_k - \sum\limits_{j=0}^{k-1} \frac{v_j}{(v_j,v_j)}(b_k, v_j)$

Example 1.6.

1. **Legender Polynomial:** Interval $[a,b] = [-1,1]$, weight function $w(x) = 1$.

   Gram-Schmidt: Starting from $1, x, x^2, \ldots$:

   $P_0(x) = 1$

   $P_1(x) = x - \frac{(x,P_0)}{(P_0,P_0)}P_0(x) = x - \frac{\int_{-1}^1 x dx}{\int_{-1}^1 dx} = x$

   $P_2(x) = x^2 - \frac{(x^2,P_0)}{(P_0,P_0)}P_0(x) - \frac{(x^2,P_1)}{(P_1,P_1)}P_1(x) =$

   $= x^2 - \frac{\int_{-1}^1 x^2 dx}{2} - \frac{\int_{-1}^1 x^3 dx}{\int_{-1}^1 x^2 dx}x = x^2 - \frac{1}{3}$

   Differential formula: $P_n(x) = \frac{(-1)^n}{2^n n!}\frac{d^n}{dx^n}\left\{\left(1-x^2\right)^n\right\}$

   Recursive formula: $P_0(x) = 1$; $P_1(x) = x$;
   $P_{n+1}(x) = \frac{2n+1}{n+1}xP_n(x) - \frac{n}{n+1}P_{n-1}(x)$

2. **Chebyshev Polynomial:** Interval $[a,b] = [-1,1]$, weight function $w(x) = \frac{1}{\sqrt{1-x^2}}$

   Direct formula: $T_n(x) = \cos(n \arccos x)$

   Recursive formula: $T_0(x) = 1$; $T_1(x) = x$;
   $T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x)$

3. **Laguerre Polynomial:** Interval $[a,b] = [0,\infty)$, weight function $w(x) = e^{-x}$

   Differential fornula: $L_n(x) = \frac{e^x}{n!}\frac{d^n}{dx^n}\left(e^{-x}x^n\right)$

   Recursive formula: $L_0(x) = 1$; $L_1(x) = 1 - x$;
   $L_{n+1}(x) = \left(\frac{2n+1-x}{n+1}L_n(x) - \frac{n}{n+1}L_{n-1}(x)\right)$

4. **Hermite Polynomial:** Interval $[a,b] = (-\infty,\infty)$, weight function $w(x) = e^{-x^2}$

   Differential formula: $H_n(x) = (-1)^n e^{x^2}\frac{d^n}{dx^n}e^{-x^2}$

   Recursive formula: $H_0(x) = 1$; $H_1(x) = 2x$;
   $H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x)$

Gaussian quadrature Recall that when the polynomial part of the error of interpolation $p(x) = (x - x_0)\ldots(x - x_n)$ is symmetrical in the domain of integration the integral is vanishes and therefore the error improves, i.e. moves to higher degree

$e(h) = \int_a^b f[x_0,...,x_n,x]\,p(x)\,dx = f[x_0,...,x_{n+1}]\int_a^b p(x)\,dx +$ $\int_a^b f[x_0,...,x_{n+1},x]\,p(x)(x - x_{n+1})\,dx$. Since the formula is valid for any x_{n+1}, one chooses x_{n+1} such that $\int_a^b p(x)(x - x_{n+1})\,dx = 0$. Actually, it doesn't depends on x_{n+1}, but on $p(x)$, that is on interpolation points.

Given $f(x)$ is $2n+2$ continuous differentiable, one choose interpolation points for $\int_a^b w(x) f(x)\,dx$ to be roots of the polynomial b_{n+1} orthogonal with respect to the weight function $w(x)$. That is, $p(x) = \frac{1}{\alpha_{n+1}}b_{n+1}$, where α_{n+1} is the leading coefficient of b_{n+1}.

For $k \leq n$ a polynomial can be represented as $P_k(x) = \sum\limits_{j=0}^{k} \alpha_j b_j(x)$ and so $(P_k(x), b_{n+1}(x)) = 0$.

Thus, we have $n+1$ points that cause the integral above to vanish, so
$e(f) = \int_a^b f[x_0,...,x_{2n+1},x]\,p(x)\prod_{j=n+1}^{2n+1}(x - x_j)dx$, where $(x - x_{n+1})\cdots(x - x_{2n+1}) = p(x)$ and therefore

$$e(f) = \frac{f^{(2n+2)}(c)}{(2n+2)!}\int_a^b p^2(x)\,w(x)\,dx$$

Theorem 1.7. Let $f(x)$ be $2n+2$ continuously differentiable function on $[a,b]$ and let $w(x)$ be a weight function. For the quadrature

$$\int f(x)\,w(x)\,dx = \sum_{j=0}^{n} A_j f(x_j)$$

1. The optimal choice of interpolation points are roots of $n+1$ orthogonal polynomial with respect to $w(x)$.

2. One find the coefficient using ether

   - By solving linear system resulting by requiring the rule be exact for $f \in \{1, x, x^2, ..., x^n\}$, or
   - Using the formula $A_j = \int_a^b l_j(x)\,w(x)\,dx = \int_a^b \prod\limits_{\substack{k=0 \\ k \neq j}}^{n} \frac{x - x_j}{x_k - x_j} w(x)\,dx$

3. The algebraic exactness of the resulting method is $2n+1$.

Algorithm:

- Find the orthogonal polynomial with respect to $w(x)$ of order $n+1$.
- Choose the roots of the orthogonal polynomial above to be interpolation points $\{x_j\}_{n=0}^n$.
- Compute the coefficients A_j