Summary of last session

-Chapter 7. Numerical Differentiation and integration

- **7.1. Numerical Differentiation and Richardson Extrapolation:**

  Numerical differentiation, Lagrange polynomial,
  Richardson extrapolation

- **7.2. Numerical Integration Based on Interpolation:**

  Newton-Cotes formula, trapezoidal formula,
  composite trapezoidal formula, Simpson’s Rule,
  composite Simpson’s Rule, general integration formula

7.3 Romberg Integration

Let us look at the Richardson Extrapolation first. We have the Taylor series for function of f around $x = 0$

$$f(h) = f(0) + hf'(0) + \frac{h^2}{2!} f''(0) + \frac{h^3}{3!} f'''(0) + \cdots$$

$$f(\frac{h}{2}) = f(0) + \frac{h}{2} f'(0) + \frac{1}{2!}\left(\frac{h}{2}\right)^2 f''(0) + \frac{1}{3!}\left(\frac{h}{2}\right)^3 f'''(0) + \cdots$$

Obviously, using $f(h)$ or $f(\frac{h}{2})$ to approximation $f(0)$, the accuracy is $O(h)$.

If we use $f_1(h) = 2f(\frac{h}{2}) - f(h)$ to approximate $f(0)$, then we have

$$f_1(h) = f(0) - \frac{h^2}{4} f''(0) - \frac{h^3}{8} f'''(0) + \cdots \qquad (1)$$

The accuracy is with the order $O(h^2)$, where we only conducted a simple calculation.

7.3 Romberg Integration

The Romberg integral is to use the composite trapezoid rule to give the inital approximation and then apply the Richardson extrapolation to improve the approximation to a required accuracy.

We suppose that an approximate value is required for the integral

$$I = \int_a^b f(x)\,dx \qquad (1)$$

The function f and the interval $[a,b]$ will remain fixed.

Recursive Trapezoid Rule

Let the trapezoid rule for I using n subintervals of width $h = \dfrac{(b-a)}{n}$ be denoted by T_n. Then

$$T_n = \frac{h}{2}\left[f(a) + f(b) + 2\sum_{i=1}^{n-1} f(a+ih) \right] = I + a_2 h^2 + a_4 h^4 + \cdots \qquad (2)$$

7.3 Romberg Integration

Using the composite trapezoid formula we get the approximation T_n, i.e. $f_1(h)$. Halfing the interval we get the T_{2n}, i.e. $f_1(\frac{h}{2})$. Then we have

$$I \approx \frac{1}{3}\left(4 f_1(\frac{h}{2}) - f_1(h)\right)$$

with accuracy O(h^4). Let

$$S_n = \frac{4}{4-1} T_{2n} - \frac{1}{4-1} T_n \qquad (3)$$

This is the formula resulted from the application of the composite trapezoid rule in each of the interval $(b-a)/n$. It is a linear extrapolation.

7.3 Romberg Integration

Similarly, we could use the composite trapezoid rule with higher accuracy for example the composite Cotes formula, then we have

$$C_n = \frac{4^2}{4^2-1} S_{2n} - \frac{1}{4^2-1} S_n \qquad (4)$$

With same procedure we can have even higher accuracy formula:

$$R_n = \frac{4^3}{4^3-1} C_{2n} - \frac{1}{4^3-1} C_n \qquad (5)$$

Generally,

$$T_m^k = \frac{4^m}{4^m-1} T_{m-1}^{k+1} - \frac{1}{4^m-1} T_{m-1}^k \qquad (m = 1, 2, 3, \cdots)$$

7.4 Gaussian Quadrature

Whether some choice of nodes are better ? The formula of Newton-Cotes uses equal spaced nodes and it is exact for polynomials of degree $\le n$. There may be better selections of the nodes which give better accuracy. **The Gauss quadrature is to select the best nodes in the interval $[a,b]$ (may not be equal spaced) and the best coefficients** c_i

$$\int_a^b f(x)dx \approx \sum_{i=0}^{n} c_i f(x_i) \tag{1}$$

to have a minimum error.

7.4 Gaussian Quadrature

The only limitation for the nodes is that they have to be in the interval while the coefficients c_i are arbitrary, which allows to determine a polynomial of degree $2n+1$. To illustrate the Gaussian quadrature, let us look at an example.

7.4 Gaussian Quadrature

Example 1: Find the Gaussian quadrature rule when $[a,b]=[-1,1]$ and $n+1=2$.

Solution : We need to find the nodes and the coefficients so that

$$\int_{-1}^{1} f(x)\,dx \approx c_0 f(x_0) + c_1 f(x_1)$$

where $f(x)$ is a polynomial of degree $\le 2n+1 = 3$, that is

$$f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3$$

$$\int (a_0 + a_1 x + a_2 x^2 + a_3 x^3)dx = a_0 \int 1dx + a_1 \int xdx + a_2 \int x^2 dx + a_3 \int x^3 dx$$

Equivalently we need

$$c_0 \cdot 1 + c_1 \cdot 1 = \int_{-1}^{1} 1dx \qquad c_0 \cdot x_0 + c_1 \cdot x_1 = \int_{-1}^{1} xdx = 0$$

$$c_0 \cdot x_0^2 + c_1 \cdot x_1^2 = \int_{-1}^{1} x^2 dx = 2/3 \qquad c_0 \cdot x_0^3 + c_1 \cdot x_1^3 = \int_{-1}^{1} x^3 dx = 0$$

The solution is $c_0 = 1, \quad c_1 = 1, \quad x_0 = -1/\sqrt{3}, \quad x_1 = 1/\sqrt{3}$

Therefore the two-point approximation formula is

$$\int_{-1}^{1} f(x)\,dx \approx f\left(-1/\sqrt{3}\right) + f\left(1/\sqrt{3}\right)$$

7.4 Gaussian Quadrature

This formula has degree of precision 3, that is, it produces the exact result for every polynomial of degree 3 or less. We have only two points but we can approximate a polynomial of degree three.

Compared to the Newton Cotes integration, it obviously has better accuracy. Since the error term of N-C integration involves $(n+1)$th derivative of the function being approximated, it is exact only when approximating any polynomial of degree less than or equal to n.

7.4 Gaussian Quadrature

N-C integration uses equally-spaced points. This restriction is convenient when the formula is combined to form the composite rules, but it can significantly decrease the accuracy of the approximation.

Gaussian quadrature chooses the points for evaluation in an optimal rather than equally spaced way. The nodes $x_1, x_2, ..., x_n$ in the interval $[a, b]$ and coefficients are chosed to minimize the error.

7.4 Gaussian Quadrature

This technique could be used to determine the nodes and coefficients for formulas that give exact results for higher-degree polynomials.

However, as the equation system is not linear, it is difficult to obtain the solutions. The key issue is to find the values of nodes. Once the nodes are determined, the coefficients can be obtained consequently.

The alternative method, instead of solving the nonlinear equation system, is to use the orthogonal polynomials.

For this, let us still look at the **example 1**.

7.4 Gaussian Quadrature

To see the relationship between the nodes and **orthogonal** polynomials, we look back the **example 1**.

Determine x_0, x_1, c_0 and c_1 in

$$\int_{-1}^{1} f(x)dx \approx c_0 f(x_0) + c_1 f(x_1) \qquad (2)$$

which has a precision of degree 3.

Solution : Let $f(x)$ be any polynomial of degree ≤ 3.

$f(x)$ always can be expressed as

$$f(x) = (a_0 + a_1 x)(x - x_0)(x - x_1) + (b_0 + b_1 x)$$

$$\int_{-1}^{1} f(x)dx = \int_{-1}^{1}(a_0 + a_1 x)(x - x_0)(x - x_1)dx + \int_{-1}^{1}(b_0 + b_1 x)dx$$

$$= c_0(b_0 + b_1 x_0) + c_1(b_0 + b_1 x_1) \qquad (3)$$

Since (2) has a precision of degree 3, we have

$$\int_{-1}^{1}(b_0 + b_1 x)dx = c_0(b_0 + b_1 x_0) + c_1(b_0 + b_1 x_1) \qquad (4)$$

7.4 Gaussian Quadrature

Comparing (4) with (3) gives

$$\int_{-1}^{1}(a_0 + a_1 x)(x - x_0)(x - x_1)dx = 0$$

for any a_0 and a_1. Specially when $a_0 = 1,\ a_1 = 0$ and $a_0 = 0$ and $a_1 = 1$, we then have

$$\begin{cases} \int_{-1}^{1}(x - x_0)(x - x_1)dx = 0 \\ \int_{-1}^{1}x(x - x_0)(x - x_1)dx = 0 \end{cases} \Rightarrow \begin{cases} \frac{2}{3} + 2x_0 x_1 = 0 \\ -\frac{2}{3}(x_0 + x_1) = 0 \end{cases} \Rightarrow x_0 = -x_1 = \frac{1}{\sqrt{3}}$$

Furthermore, let $f_1(x) = 1,\ f_2(x) = x$, and from (2) we have

$$\int_{-1}^{1} f(x)dx \approx c_0 f(x_0) + c_1 f(x_1) \quad (2)$$

$$\begin{cases} \int_{-1}^{1}1dx = 2 = c_0 + c_1 \\ \int_{-1}^{1}xdx = 0 = c_0 \frac{1}{\sqrt{3}} - c_1 \frac{1}{\sqrt{3}} \end{cases} \Rightarrow c_0 = c_1 = 1$$

7.4 Gaussian Quadrature

$$\int_a^b f(x)w(x)dx \approx \sum_{i=0}^{n} c_i f(x_i) \quad (2)$$

In general, any polynomial of degree $\leq 2n+1$, $p_{2n+1}(x)$, may be written as

$$p_{2n+1}(x) = q(x)\omega_{n+1}(x) + r(x) \qquad (6)$$

where $q(x)$ and $r(x)$ are polynomial of degree $\leq n$, and $\omega_{n+1}(x) = \prod_{k=0}^{n}(x - x_k)$.

Substitute (6) into (2), and because (2) is exact for $r(x)$, we have

$$\int_a^b w(x)q(x)\omega_{n+1}(x)dx = 0 \qquad (7)$$

where $w(x)$ is the weight function. For any $q(x)$ (of degree $\leq$ n), (7) is called the orthogonal condition. Specially, let $q(x) = 1, x, \ldots, x^{n-1}, x^n$, substitute them into (7) respectively, and get an n+1−equation system $\Rightarrow$ obtain the values for $\{x_k\}$. Then,

we can solve

$$\begin{cases} c_0 + c_1 + c_2 + \ldots + c_n = \int_a^b w(x) \cdot 1 \cdot dx \\ c_0 x_0 + c_1 x_1 + c_2 x_2 + \ldots + c_n x_n = \int_a^b w(x) \cdot x \cdot dx \\ \vdots \\ c_0 x_0^n + c_1 x_1^n + c_2 x_2^n + \ldots + c_n x_n^n = \int_a^b w(x) \cdot x^n \cdot dx \end{cases} \Rightarrow c_0, c_1, c_2, \ldots, c_n$$

(It can be proved that the nodes are the zeros of the orthogonal polynomial of degree $n+1$.)

7.4 Gaussian Quadrature

-Back to general integration formula

More general integration formula is of the type

$$\int_a^b f(x)w(x)dx \approx \sum_{i=0}^{n} A_i f(x_i) \qquad (8)$$

where *w(x)* can be any fixed positive weight function. The only modification necessary to the coefficient is

$$A_i = \int_a^b w(x) \prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{x - x_j}{x_i - x_j} dx \qquad (10)$$

The case when $w(x) \equiv 1$ is of special importance. Because there are $n+1$ coefficients A_i and $n+1$ nodes x_i, the formula (8) is exact for polynomials of degree $\leq 2\text{n}+1$.

7.4 Gaussian Quadrature

Summary of above, there are $n+1$ coefficients A_i and $n+1$ nodes x_i.

It can be proved that the nodes $x_0, x_1, \ldots, x_n$ are the zeros of a nonzero polynomial of degree $n+1$ that is $w-$orthogonal to any polynomial of degree no more than n.

The coefficients A_i can also be recovered from the following relations if we know the n + 1 nodes.

$$\begin{cases} \sum_{i=0}^{n} A_i = \int_a^b w(x)\,dx \\ \sum_{i=0}^{n} A_i x_i = \int_a^b w(x)\,x\,dx \\ \quad\vdots \\ \sum_{i=0}^{n} A_i x_i^n = \int_a^b w(x)\,x^n\,dx \end{cases} \qquad (11)$$

Another way to determine the coefficients is using the formula (10)

7.4 Gaussian Quadrature

In Chapter 6, the orthogonal polynomials were introduced. A related polynomial to this chapter is the **Legendre polynomial** which has the following properties:

1. for every n, $q_n(x)$ is a polynomial of degree n
2. for the polynomial of degree smaller than n, $\int_{-1}^{1} q(x) q_n(x)\,dx = 0$

The first several polynomials are

$$q_0(x) = 1, \quad q_1(x) = x, \quad q_2(x) = x^2 - \frac{1}{3}, \quad q_3(x) = x^3 - \frac{3}{5}x,$$

$$q_4(x) = x^4 - \frac{6}{7}x^2 + \frac{3}{35}$$

Let us look at an example which uses this polynomial to find the **Guass - Legendre** quadrature.

7.4 Gaussian Quadrature

Example 2 Find the Gaussian formula for $[-1,1]$, $w(x)=1$, and $n=2$.

Solution: (n + 1 nodes and degree 2n + 1) The Legendre polynomial is orthogonal to $w(x)=1$ in $[-1,1]$. When $n=2$ there are 3 nodes which are the zeros of the Legendre polynomial of degree 3

$$q_3(x)=x^3-(3/5)x$$

The roots 0 and $\pm\sqrt{3/5}$ of this polynomial are the nodes and the coefficients then can be calculated using (11)

$$\begin{cases} A_0+A_1+A_2=\int_{-1}^{1} 1dx=2 \\ -A_0(\sqrt{3/5})+A_2(\sqrt{3/5})=\int_{-1}^{1} xdx=0 \\ (3/5)(A_0+A_2)=\int_{-1}^{1} x^2dx=2/3 \end{cases} \Rightarrow \begin{cases} A_0=5/9 \\ A_1=8/9 \\ A_2=5/9 \end{cases}$$

Therefore the Gaussian formula is

$$\int_{-1}^{1} f(x)dx \approx (5/9)f\left(-\sqrt{3/5}\right)+(8/9)f(0)+(5/9)f\left(\sqrt{3/5}\right)$$

The constants, A_0, A_1, and A_2 may also be calculated using (10).

7.4 Gaussian Quadrature

Example Find the Gaussian formula for $[-1,1]$, $w(x)=1$, and $n=2$.

Solution : The constants, $A_0, A_1,$ and A_2 may be calculated using (10).

$$A_i = \int_a^b w(x) \prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{x-x_j}{x_i-x_j}\, dx \tag{10}$$

where $x_0 = -\sqrt{3/5}, x_1 = 0, x_2 = \sqrt{3/5}$.

$$A_0 = \int_{-1}^{1} 1 \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} dx = \frac{2/3}{6/5} = \frac{5}{9}$$

$$A_1 = \int_{-1}^{1} 1 \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} dx = \frac{-8/15}{-3/5} = \frac{8}{9}$$

$$A_2 = \int_{-1}^{1} 1 \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} dx = \frac{2/3}{6/5} = \frac{5}{9}$$

For well behaved integrands, modest accuracy is obtained with only a few function evaluations using Gaussian formulas, and even more accuracy can be obtained by using some of the high-order formulas.

7.4 Gaussian Quadrature

The Gaussian formula for $[-1,1]$ and $w(x)=\dfrac{1}{\sqrt{1-x^2}}$ is

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

which is called the **Guassian - Chebyshev** quadrature formula.

We have known that the orthogonal polynomials on $[-1,1]$ with weight $\dfrac{1}{\sqrt{1-x^2}}$ are Chebyshev polynomials, thus the Guassian nodes for the above quadrature formula are the zeros of the Chebyshev polynomial of degree $n+1$, which are

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

It can be derived that $A_k=\dfrac{\pi}{n+1}$. For convenience, we give the following Guassian-Chebyshev quadrature formula with n nodes:

$$\int_{-1}^{1}\frac{f(x)}{\sqrt{1-x^2}}dx \approx \frac{\pi}{n}\sum_{k=1}^{n} f(x_k), \quad x_k=\cos\frac{(2k-1)}{2n}\pi \quad (k=1,\cdots,n).$$

The error term of this formula can be obtained by

$$R[f]=\frac{2\pi}{2^{2n}(2n)!}f^{(2n)}(\eta), \qquad \eta\in(-1,1).$$

7.4 Gaussian Quadrature

Example Use the Guassian-Chebyshev quadrature formula with 5 nodes ($n = 5$) to calculate

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

Solution Here $f(x)=e^x, f^{(2n)}(x)=e^x$, the Guassian-Chebyshev quadrature formula with $n = 5$ becomes

$$I = \int_{-1}^{1} \frac{e^x}{\sqrt{1-x^2}} dx \approx \frac{\pi}{5} \sum_{k=1}^{5} e^{\cos\frac{2k-1}{10}\pi} = 3.977463,$$

with the error

$$R[f] \le \frac{\pi}{2^9 10!} e \le 4.6 \times 10^{-9}.$$

Example

Use different methods to approximate

$$I = \int_0^1 \frac{\sin x}{x} dx$$

$f(0) = 1, \ f(1) = 0.8414709$

Solution : (1) by the composite trapezoidal formula, after 10 times of halfing the interval and use 1025 function values, we finally get the exact result

$$I = 0.9460831$$

(2) by the Romberg method, after 3 times of halfing and use 9 function values, and reach the same result

k	T_{2^k}	$S_{2^{k-1}}$	$C_{2^{k-2}}$	$R_{2^{k-3}}$
0	0.9207355			
1	0.9397933	0.9461459		
2	0.9445135	0.9460869	0.9460830	
3	0.9456909	0.9460834	0.9460831	0.9460831

Example*

(3) by Gauss Quadrature, we use 3 nodes formula.

Do a transformation first

$$x = \frac{1}{2}(t+1)$$

change the interval from [0,1] to [-1, 1], and

$$\mathrm{I} = \int_0^1 \frac{\sin x}{x}dx = \int_{-1}^1 \frac{\sin\frac{1}{2}(t+1)}{(t+1)}dt$$

Then $\mathrm{I} \approx 0.5555556 \times \dfrac{\sin\frac{1}{2}(-0.7745967+1)}{-0.7745967+1} + 0.8888889 \times \dfrac{\sin\frac{1}{2}}{0+1}$

$$+0.5555556 \times \frac{\sin\frac{1}{2}(0.7745967+1)}{0.7745967+1} = 0.9460831$$

We only use 3 function values and reache the same value.

Exercises

$Ex1$. Determine the constants A, B, C, and α so as to obtain a quadrature formula

$$\int_{-2}^{2} f(x)dx \approx Af(-\alpha) + Bf(0) + Cf(\alpha)$$

which has degree of precision as high as possible.

Ex2. Approximate the following integral using Gauss Quadrature.

(1) $\int_0^{\pi/2} \sqrt{1 - \frac{1}{2}\sin^2 t}\, dt$ (with 3 points formula)

(2) $\int_{-1}^{1} \frac{x^2}{\sqrt{1-x^2}} \mathrm{dx}$ (with 3 points formula)

Ex3. Use the Romberg method to approximate $I = \int_0^1 x^{3/2} dx, m = 5.$

(Precision to 6 decimal places)