Summary of last session

-Chapter 6. Approximating Function

- **6.4. Best Approximation---Least Squares Method:**

Discrete least square approximation

Orthogonal polynomial and least squares approximation

Chapter Seven

Numerical Differentiation and Integration

Chapter Seven
Numerical Differentiation and Integration

The purpose of this chapter:

Fundamental calculus:

$$I=\int_a^b f(x)dx=F(x)\big|_a^b=F(b)-F(a)$$

Difficulties and limitations:

1. $F(x)$ can't be expressed in a finite form;

$$\int_0^1 \frac{\sin x}{x}dx,\qquad \int_0^1 e^{-x^2}dx,\qquad \int_0^1 \frac{1}{\sqrt{1+x^4}}dx$$

2. $F(x)$ is too complicated;

$$\int_{\sqrt{3}}^{\pi}\frac{1}{1+x^4}dx=\left\{\frac{1}{4\sqrt{2}}\ln\frac{x^2+\sqrt{2}x+1}{x^2-\sqrt{2}x+1}+\frac{1}{2\sqrt{2}}\left[\arctan(\sqrt{2}x+1)+\arctan(\sqrt{2}x-1)\right]\right\}\Bigg|_{\sqrt{3}}^{\pi}$$

3. $f(x)$ is given at a few points.

we need to find ways estimating the derivative or an integral of $f(x)$

Chapter Seven

7.1 Numerical Differentiation and Richardson Extrapolation

7.2 Numerical Integration Based on Interpolation

7.3 Gaussian Quadrature

7.4 Romberg Integration

7.1 Numerical Differentiation and Richardson Extrapolation

- Numerical differentiation

We use the difference to approximate the differentiation, such that:

$$f'(x) \approx \frac{1}{h}\left[f(x+h) - f(x)\right] \qquad (1)$$

To assess the error, we consider the Taylor's Theorem:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(\xi) \qquad (2)$$

Rearranging the equation, we get:

$$f'(x) = \frac{1}{h}\left[f(x+h) - f(x)\right] - \frac{h}{2}f''(\xi) \qquad (3)$$

where ξ is a point between x and $x+h$.

The h-*term* in the error makes the entire expression converge to 0 as h approaches to 0. The rapidity of this convergence will depend on the power of h.

7.1 Numerical Differentiation and Richardson Extrapolation

$$f'(x) \approx \frac{1}{h}\left[f(x+h) - f(x)\right] \quad (1)$$

Example 1 Using formula (1) to compute the derivative of

$$f(x) = \cos x \text{ at } x = \frac{\pi}{4} \text{ with } h = 0.01,$$

what is the result and accuracy?

Solution: Using a calculator, we find

$$f'(x) \approx \frac{1}{h}\left[f(x+h) - f(x)\right]$$

$$= \frac{1}{0.01}\left[0.700000476 - 0.707106781\right]$$

$$= -0.71063051$$

The error can be estimated by

$$\left|\frac{h}{2} f''(\xi)\right| = 0.005\left|\cos \xi\right| \le 0.005$$

7.1 Numerical Differentiation and Richardson Extrapolation

The actual error is

$$-\sin\frac{\pi}{4}+0.71063051=0.003523729$$

The term $\frac{h}{2}f''(x)$ in (3) we omitted in (1) is called Truncation Error.

To compute $f'(x)$ accurately, it is necessary that h must be small because the error is proportional to h.

The precision of a differentiation formula is often judged simply by the power of h in the error term.

To enhance the precision, we can simply consider

$$f'(x)\approx\frac{1}{2h}\left[f(x+h)-f(x-h)\right] \qquad (4)$$

7.1 Numerical Differentiation and Richardson Extrapolation

This is derived from two cases of Taylor's Theorem:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{3!} f'''(\xi_1) \qquad (5)$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2} f''(x) - \frac{h^3}{3!} f'''(\xi_2) \qquad (6)$$

Subtracting and rearranging, we obtain

$$f'(x) = \frac{1}{2h}\left[f(x+h) - f(x-h)\right] - \frac{h^2}{12}\left[f'''(\xi_1) + f'''(\xi_2)\right] \qquad (7)$$

This is a better result than (3) because we have h^2 in error term.

$$f'(x) = \frac{1}{h}\left[f(x+h) - f(x)\right] - \frac{h}{2} f''(\xi) \qquad (3)$$

7.1 Numerical Differentiation and Richardson Extrapolation

If we assume that f''' is continuous, we have

$$f'''(\xi)=\frac{1}{2}\left[f'''(\xi_1)+f'''(\xi_2)\right]$$

and subsequently we have

$$f'(x)=\frac{1}{2h}\left[f(x+h)-f(x-h)\right]-\frac{h^2}{6}f'''(\xi) \qquad (8)$$

Extending equations (5) and (6) by one more term and adding the equations and rearranging, we have

$$f''(x)=\frac{1}{h^2}\left[f(x+h)-2f(x)+f(x-h)\right]-\frac{h^2}{12}f^{(4)}(\xi) \qquad (9)$$

for some $\xi\in(x-h,\ x+h)$.

7.1 Numerical Differentiation and Richardson Extrapolation
- Lagrange Polynomial

Lagrange Polynomial

Suppose that we have $n+1$ values of a function f at points $x_0, x_1, \cdots, x_n$, a polynomial that interpolates f at the nodes x_i can be written in the following form:

$$L_n(x) = \sum_{i=0}^{n} l_i(x) f(x_i)$$

where $l_i(x)$ has the property

$$l_i(x) = \delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

and the form

$$l_i(x) = \frac{(x-x_0)(x-x_1)\cdots(x-x_{i-1})(x-x_{i+1})\cdots(x-x_n)}{(x_i-x_0)(x_i-x_1)\cdots(x_i-x_{i-1})(x_i-x_{i+1})\cdots(x_i-x_n)} = \prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{(x-x_j)}{(x_i-x_j)}$$

Therefore, at $x = x_j$

$$L_n(x_j) = \sum_{i=0}^{n} l_i(x_j) f(x_i) = \sum_{i=0}^{n} \delta_{ij} f(x_i) = f(x_j)$$

It is called the Lagrange Polynomial and is exact equal to f at x_j.

7.1 Numerical Differentiation and Richardson Extrapolation

We have learnt that

$$f(x)=L_n(x)+R_n(x)=\sum_{i=0}^{n} f(x_i)l_i(x)+\frac{f^{(n+1)}(\xi)}{(n+1)!}\prod_{i=0}^{n}(x-x_i) \quad (10)$$

The error is $$R_n(x)=\frac{f^{(n+1)}(\xi)}{(n+1)!}\prod_{i=0}^{n}(x-x_i).$$

and $$R_n'(x)=\frac{f^{(n+1)}(\xi)}{(n+1)!}\sum_{i=0}^{n}\prod_{j=0,\, j\neq i}^{n}(x-x_j)+\frac{1}{(n+1)!}\prod_{i=0}^{n}(x-x_i)\frac{d}{dx}f^{(n+1)}(\xi).$$

Therefore **the differentiation formula with error term using the Lagrange polynomial** at point $x=x_\alpha$ is

$$f'(x_\alpha)=\sum_{i=0}^{n} f(x_i)l_i'(x_\alpha)+\frac{1}{(n+1)!}f^{(n+1)}(\xi_{x_\alpha})\sum_{i=0}^{n}\prod_{\substack{j=0\\ j\neq i}}^{n}(x_\alpha-x_j) \qquad (11)$$

This formula is particularly well suited for nonequally spaced nodes. This is called an $(n+1)$-point formula.

$$f'(x_\alpha) = \sum_{i=0}^{n} f(x_i) l_i'(x_\alpha) + \frac{1}{(n+1)!} f^{(n+1)}(\xi_{x_\alpha}) \sum_{i=0}^{n} \prod_{\substack{j=0 \\ j\neq i}}^{n} (x_\alpha - x_j) \quad (11)$$

Example 2 Give the explicit form of equation (11) when $n = 2$ and $\alpha = 1$

Solution : The three basic functions for Lagrange interpolation are

$$l_0(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)}$$

$$l_1(x) = \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)}$$

$$l_2(x) = \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)}$$

The derivatives are

$$l_0'(x) = \frac{2x - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)}$$

$$l_1'(x) = \frac{2x - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)}$$

$$l_2'(x) = \frac{2x - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)}$$

Evaluating at x_1, we obtain

$$l_0'(x_1) = \frac{x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)}$$

$$l_1'(x_1) = \frac{2x_1 - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)}$$

$$l_2'(x_1) = \frac{x_1 - x_0}{(x_2 - x_0)(x_2 - x_1)}$$

7.1 Numerical Differentiation and Richardson Extrapolation
- Lagrange Polynomial

Thus, the numerical differentiation formula with its error term

$$f'(x_1) = f(x_0)\frac{x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)} + f(x_1)\frac{2x_1 - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)} + f(x_2)\frac{x_1 - x_0}{(x_2 - x_0)(x_2 - x_1)} + \frac{1}{6} f'''(\xi_{x_1})(x_1 - x_0)(x_1 - x_2) \qquad (12)$$

$$f'(x) = \frac{1}{2h}\left[f(x+h) - f(x-h)\right] - \frac{h^2}{6} f'''(\xi) \quad (8)$$

This is so-called three-point formula with $x_a = x_1$. If the nodes are equally spaced, i.e. $x_0 = x_1 - h$ and $x_2 = x_1 + h$, then we have

$$f'(x_1) = f(x_1 - h)\left(\frac{-1}{2h}\right) + f(x_1 + h)\left(\frac{1}{2h}\right) - \frac{1}{6} f'''(\xi_{x_1}) h^2$$

This is the same as what we have derived in (8).

$$f'(x)=\frac{1}{2h}\left[f(x+h)-f(x-h)\right]-\frac{h^2}{6}f'''(\xi) \quad (8)$$

Example 3 Values for $f(x)=xe^x$ are given in the following table.

x	1.8	1.9	2.0	2.1	2.2
$f(x)$	10.889365	12.703199	14.778112	17.148957	19.855030

Since $f'(x)=(x+1)e^x$, we have $f'(2.0)=22.167168$. Approximate $f'(2.0)$ using the various three-point formula.

Solution let $h=0.1,\ x_0=1.9,\ x_1=2.0,\ x_2=2.1$

$$f'(2.0)=\frac{1}{0.2}[f(2.1)-f(1.9)]=\frac{1}{0.2}[17.148957-12.703199]=22.228790;$$

or let $h=0.2,\ x_0=1.8,\ x_1=2.0,\ x_2=2.2$

$$f'(2.0)=\frac{1}{0.4}[f(2.2)-f(1.8)]=\frac{1}{0.2}[19.855030-10.889365]=22.414163$$

7.1 Numerical Differentiation and Richardson Extrapolation

-Richardson Extrapolation

Richardson Extrapolation

Richardson extrapolation is used to obtain more accuracy out of some numerical formulas. Assuming that $f(x)$ is represented by its Taylor series

$$f(x+h)=\sum_{k=0}^{\infty}\frac{1}{k!}h^k f^{(k)}(x) \qquad (13)$$

$$f(x-h)=\sum_{k=0}^{\infty}\frac{1}{k!}(-1)^k h^k f^{(k)}(x) \qquad (14)$$

If the second equation is subtracted from the first, all terms with an even value of k will cancel, so that

$$f(x+h)-f(x-h)=2hf'(x)+\frac{2}{3!}h^3 f'''(x)+\frac{2}{5!}h^5 f^{(5)}(x) +\ldots$$

7.1 Numerical Differentiation and Richardson Extrapolation

-Richardson Extrapolation

Then the differentiation of f is

$$f'(x) \approx \frac{1}{2h}\left[f(x+h) - f(x-h)\right] \quad (4)$$

$$f'(x) = \frac{1}{2h}\left[f(x+h) - f(x-h)\right]$$

$$-\left[\frac{1}{3!}h^2 f^{(3)}(x) + \frac{1}{5!}h^4 f^{(5)}(x) + \frac{1}{7!}h^6 f^{(7)}(x) + \ldots\right]$$

The equation has the form

$$L = \phi(h) + a_2 h^2 + a_4 h^4 + a_6 h^6 + \ldots \qquad (15)$$

where L stands for $f'(x)$ and $\phi(h)$ stands for the numerical differentiation formula (4); that is,

$$\phi(h) = \frac{1}{2h}\left[f(x+h) - f(x-h)\right]$$

The error is given by the series $a_2h^2 + a_4h^4 + a_6h^6 + \ldots$, so we **therefore look for a way of eliminating the dominant term**, a_2h^2.

7.1 Numerical Differentiation and Richardson Extrapolation

-Richardson Extrapolation

$$L = \phi(h) + a_2 h^2 + a_4 h^4 + a_6 h^6 + \ldots \qquad (15)$$

Write out Equation (15) with h replaced by $h/2$:

$$L = \varphi\left(\frac{h}{2}\right) + a_2\frac{h^2}{4} + a_4\frac{h^4}{16} + a_6\frac{h^6}{64} + \ldots \qquad (16)$$

Eliminate $a_2 h^2$ from Equations (15) and (16) by multiplying the latter by 4 and subtracting the former from it. Thus, we have

$$L = \frac{4}{3}\varphi\left(\frac{h}{2}\right) - \frac{1}{3}\varphi(h) - a_4\frac{h^4}{4} - 5a_6\frac{h^6}{16} - \ldots \qquad (17)$$

Equation (17) embodies the first step in Richardson extrapolation. **A simple combination of $\varphi(h)$ and $\varphi(h/2)$ ends an estimation with accuracy $O(h^4)$.**

7.1 Numerical Differentiation and Richardson Extrapolation

-Richardson Extrapolation

$$L = \frac{4}{3}\phi\left(\frac{h}{2}\right) - \frac{1}{3}\phi(h) - a_4\frac{h^4}{4} - 5a_6\frac{h^6}{16} - \dots \quad (17)$$

We can repeatedly do the substracting to increase the precision.

Let $$\psi(h) = \frac{4}{3}\phi\left(\frac{h}{2}\right) - \frac{1}{3}\phi(h)$$

Then from (17) we have

$$L = \psi(h) + b_4 h^4 + b_6 h^6 + \dots$$

$$L = \psi(h/2) + b_4 h^4/16 + b_6 h^6/64 + \dots$$

Now eliminate $b_4 h^4$ from above equations by multiplying the latter by 16 and subtracting the former from it. Thus, we have

$$L = \frac{16}{15}\psi\left(\frac{h}{2}\right) - \frac{1}{15}\psi(h) - b_6\frac{h^6}{20} - \dots \quad (18)$$

7.1 Numerical Differentiation and Richardson Extrapolation

-Richardson Extrapolation

$$L = \frac{16}{15}\psi\left(\frac{h}{2}\right) - \frac{1}{15}\psi(h) - b_6\frac{h^6}{20} - \ldots \qquad (18)$$

Again, we can let

$$\theta(h) = \frac{16}{15}\psi\left(\frac{h}{2}\right) - \frac{1}{15}\psi(h)$$

in equation (18) so that

$$L = \theta(h) + c_6 h^6 + c_8 h^8 + \ldots$$

In the same manner, we have

$$L = \theta(h/2) + c_6 h^6/64 + c_8 h^8/256 + \ldots$$

$$L = \frac{64}{63}\theta\left(\frac{h}{2}\right) - \frac{1}{63}\theta(h) - c_8\frac{3h^8}{252} - \ldots$$

As a matter of fact, any number of steps can be carried out to obtain formulas of increasing precision.

Example 3 Values for $f(x) = xe^x$ are given in the following table.

x	1.8	1.9	2.0	2.1	2.2
$f(x)$	10.889365	12.703199	14.778112	17.148957	19.855030

Example 4 Approximate $f'(x)$ using the Richardson extrapolation for example 3.

Solution $\phi\left(\frac{h}{2}\right)$ is the value of $f'(2.0)$ when $h = 0.1$, which is 22.228790

$\phi(h)$ is the value of $f'(2.0)$ when $h = 0.2$, which is 22.414163

The improved value for $f'(2.0)$ can be obtained using the formula

$$\frac{4}{3}\phi\left(\frac{h}{2}\right) - \frac{1}{3}\phi(h) = \frac{4}{3}\times 22.228790 - \frac{1}{3}\times 22.414163$$

$$= 29.638386 - 7.4713876$$

$$= 22.166995$$

The exact value from the function correct to six dicemal places for $f'(2.0)$ is 22.167168, so the resulting value is obviously improved.

7.2 Numerical Integration Based on Interpolation

Facing the difficulties where the antiderivative of the function $f\,(x)$ is not simple or not easy to be found, a powerful strategem in numerically computing the integral

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

is to replace f by a function g that approximates f well and is easily integrated. That is

$$\int_a^b f(x)dx \approx \int_a^b g(x)dx$$

For example, g can be a polynomial that interpolates to f, or a polynomial by truncating a Taylor series. It is desirable to have general procedures that require only evaluations of the integrand such as the methods based on interpolation of function f.

7.2 Numerical Integration Based on Interpolation

- Newton-Cotes formula

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

Integration via Polynomial Interpolation - Newton-Cotes Formula

We use the Lagrange interpolation to approximate the function f and to evaluate the integral (1).

Select nodes $x_0, x_1, x_2, \ldots, x_n$ in $[a,b]$ and set up a Lagrange interpolation. Define

$$l_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j} \qquad (0 \leq i \leq n)$$

These are the fundamental polynomials for interpolation. The polynomial of degree at most n that interpolates f at the nodes is

$$p(x) = L_n(x) = \sum_{i=0}^{n} f(x_i) l_i(x) \qquad (2)$$

7.2 Numerical Integration Based on Interpolation

- Newton-Cotes formula

Then, the integration can be simply written as

$$I=\int_a^b f(x)\,dx \approx I_n=\int_a^b L_n(x)dx=\sum_{i=0}^{n} f(x_i)\int_a^b l_i(x)dx$$

In this way, we construct the following integration formula :

$$I=\int_a^b f(x)dx \approx I_n=\sum_{i=0}^{n} A_i f(x_i) \qquad (3)$$

where

$$A_i=\int_a^b l_i(x)\,dx \qquad (4)$$

This is called integration via polynomial interpolation, and the error term

$$R[f]=I-I_n=\int_a^b \left(f(x)-L_n(x)\right)dx=\int_a^b \frac{f^{(n+1)}(\xi_x)}{(n+1)!}\prod_{i=0}^{n}(x-x_i)dx$$

Particularly, it is called **Newton-Cotes formula** if the nodes are equally spaced.

7.2 Numerical Integration Based on Interpolation

- Newton-Cotes formula – trapezoidal formula

Trapezoid Rule

If $n=1$ and $x_0 = a$ and $x_1 = b$, the fundamental funtions are

$$l_0(x) = \frac{b-x}{b-a} \quad \text{and} \quad l_1(x) = \frac{x-a}{b-a}$$

So that :

$$A_0 = \int_a^b l_0(x)dx = \frac{1}{2}(b-a) = \int_a^b l_1(x)dx = A_1$$

and the corresponding formula is

$$\int_a^b f(x)dx \approx \frac{b-a}{2}[f(b)+f(a)] \qquad (5)$$

This is **the Trapezoid Rule**.

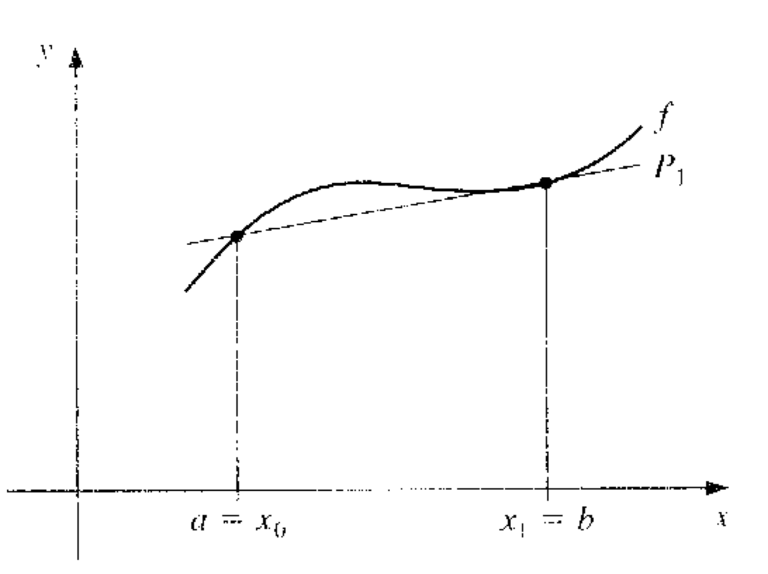
7.2 Numerical Integration Based on Interpolation

- Newton-Cotes formula – trapezoidal formula

The error term of this formula can be determined by integrating the error term in the polynomial approximation

$$R_T = \int_a^b (f(x) - p_1(x))dx = \int_a^b \frac{f^{(n+1)}(\xi_x)}{(n+1)!} \prod_{i=0}^{n} (x - x_i)dx$$

$$= \int_a^b \frac{1}{2} f''(\xi_x)(x-a)(x-b)dx = -\frac{1}{12}(b-a)^3 f''(\xi) \text{ , } \xi \in (a,b) \quad (6)$$



7.2 Numerical Integration Based on Interpolation

- Newton-Cotes formula

Example 1

If we take $n=2$ and $[a, b]=[0, 1]$ in the Newton- Cotes procedure, we obtain an formula

$$\int_0^1 f(x)\,dx \approx \frac{1}{6}f(0)+\frac{2}{3}f\left(\frac{1}{2}\right)+\frac{1}{6}f(1) \qquad (9)$$

Derive this rule by using formula (3): $\int_a^b f(x)\,dx \approx \sum_{i=0}^{n} A_i f(x_i)$.

Solution: The three fundamental polynomials for nodes 0, 0.5, 1 are

$$l_0(x)=2(x-\frac{1}{2})(x-1),\ l_1(x)=-4x(x-1),\ l_2(x)=2x(x-\frac{1}{2})$$

Then by (4) we have

$$A_i=\int_a^b l_i(x)\,dx \qquad (4)$$

$$A_0=\int_0^1 l_0(x)\,dx=\frac{1}{6},\quad A_1=\int_0^1 l_1(x)\,dx=\frac{2}{3},\quad A_2=\int_0^1 l_2(x)\,dx=\frac{1}{6}$$

7.2 Numerical Integration Based on Interpolation

- Newton Cotes - Simpson's Rule

Simpson's Rule results from integrating over $[a, b]$ the second Lagrange polynomial with nodes $x_0 = a,\ x_2 = b,$ and $x_1 = a + h,$ where $h = (b-a)/2.$ Therefore

$$\int_a^b f(x)\,dx \approx \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right] \qquad (10)$$

The error term associated with Simpson's rule is

$$R_S = \frac{1}{3!}\int_{\mathrm{a}}^{\mathrm{b}} (\mathrm{x}-\mathrm{a})(\mathrm{x}-\mathrm{b})(\mathrm{x}-\frac{a+b}{2}) f'''(\xi_x)\,dx = -\frac{1}{90}\left[\frac{(b-a)}{2}\right]^5 f^{(4)}(\xi) \qquad (11)$$

for some $\xi \in (a, b)$.

Since the error term involves the fourth derivative of f, Simpson's rule gives exact results when applied to any polynomial of degree three or less.

7.2 Numerical Integration Based on Interpolation

- Newton Cotes - Simpson's Rule

Example 2 The trapezoidal rule for a function f on the interval [0, 2] is

$$\int_0^2 f(x)\,dx \approx f(0) + f(2)$$

and the Simpson rule for f on [0, 2] is

$$\int_0^2 f(x)\,dx \approx \frac{1}{3}[f(0) + 4f(1) + f(2)].$$

The results for some elementary functions are summarized in the Table. It is noticed that in each instance Simpson rule is significantly better.

f(x)	x^2	x^4	*1/(x+1)*	*Sq(1+x²)*	sin*x*	e^x
Exact value	2.667	6.400	1.099	2.958	1.416	6.389
Trapezoidal	4.000	16.000	1.333	3.326	0.909	8.389
Simpson's	2.667	6.667	1.111	2.964	1.425	6.421

7.2 Numerical Integration Based on Interpolation

- Newton-Cotes formula – composite trapezoidal

If we further partition the interval with uniform spacing $h = \dfrac{(b-a)}{n}$ and $x_i = a + ih,$ we obtain the **composite trapezoid** rule such that

$$\int_a^b f(x)dx \approx \frac{h}{2}\left[f(a) + 2\sum_{i=1}^{n-1} f(a+ih) + f(b) \right] \qquad (7)$$

and the error term can be obtained from summing the error term by (6) for every subinterval and using the fact that there exists a point ξ in $[a,b]$ for which the average value of $f''(\xi_i)$ can be obtained by

$$f''(\xi) = \frac{1}{n}\sum_{i=1}^{n} f''(\xi_i) \quad \text{where } \xi_i \in (x_{i-1},\ x_i)$$

$$R = \sum_{i=1}^{n} \frac{-1}{12} h^3 f''(\xi_i) = -\frac{1}{12} h^3 n f''(\xi) = -\frac{1}{12}(b-a) h^2 f''(\xi) \qquad (8)$$

where $\xi \in (a,b)$.

$$R_T = -\frac{1}{12}(b-a)^3 f''(\xi) \qquad (6)$$

7.2 Numerical Integration Based on Interpolation

- Newton Cotes - Composite Simpson's Rule

Composite Simpson's Rule

Consider an even number of subintervals (a composite Simpson's rule often uses) and let n be even, and set

$$x_i = a + ih \qquad h = \frac{(b-a)}{n} \qquad (0 \le i \le n)$$

Then $$\int_a^b f(x)dx = \int_{x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + \ldots + \int_{x_{n-2}}^{x_n} f(x)dx = \sum_{i=1}^{n/2} \int_{x_{2i-2}}^{x_{2i}} f(x)dx$$

7.2 Numerical Integration Based on Interpolation

- Newton Cotes -Composite Simpson's Rule

Now apply the Simpson's rule (10) to each subinterval, and we have

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

The right-hand side of this formula should be computed as follows, to avoid repetition of terms:

$$\int_a^b f(x)\,dx \approx \frac{h}{3}\left[f(x_0)+2\sum_{i=2}^{n/2}f(x_{2i-2})+4\sum_{i=1}^{n/2}f(x_{2i-1})+f(x_n)\right] \quad (12)$$

The error term for this formula is

$$R_S = -\frac{1}{90}\left[\frac{(b-a)}{2}\right]^5 f^{(4)}(\xi) \quad (11)$$

$$R = -\frac{1}{180}(b-a)h^4 f^{(4)}(\xi) \quad (13)$$

for some $\xi \in (a,b)$.

$$\int_a^b f(x)\,dx \approx \frac{b-a}{6}\left[f(a)+4f\left(\frac{a+b}{2}\right)+f(b)\right] \quad (10)$$

7.2 Numerical Integration Based on Interpolation

- Newton Cotes

Example 4 Calculate the integration using Trapezoidal rule and Simpson rule and estimate the errors.

$$I = \int_0^1 e^x dx$$

$$\int_a^b f(x)dx \approx \frac{b-a}{2}[f(b)+f(a)] \quad (5)$$

Solution: by the Trapezoidal formula (5)

$$I \approx \frac{1}{2}(e^0 + e^1) = 1.85914$$

$$R_T = -\frac{1}{12}(b-a)^3 f''(\xi) \quad (6)$$

and the truncation error is $|R_1| = \frac{1}{12}|f''(\xi)| \le \frac{e}{12} = 0.22652$

by the Simpsonl formula (10)

$$\int_a^b f(x)dx \approx \frac{b-a}{6}\left[f(a)+4f\left(\frac{a+b}{2}\right)+f(b)\right] \quad (10)$$

$$I \approx \frac{1}{6}(e^0 + 4e^{1/2} + e^1) = 1.71886$$

$$R_S = -\frac{1}{90}\left[\frac{(b-a)}{2}\right]^5 f^{(4)}(\xi) \quad (11)$$

and the truncation error is $|R_2| = \frac{1}{2880}|f^{(4)}(\xi)| \le \frac{e}{2880} = 0.00095$

7.2 Numerical Integration Based on Interpolation

- Newton Cotes – general integration formula*

More general integration formula is of the type

$$\int_a^b f(x)w(x)dx \approx \sum_{i=0}^{n} A_i f(x_i) \tag{14}$$

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

$$A_i = \int_a^b l_i(x)w(x)dx \tag{15}$$

Let's look at an example

Example 3 Find a formula

$$\int_{-\pi}^{\pi} f(x)\cos x dx \approx A_0 f\left(-\frac{3}{4}\pi\right) + A_1 f\left(-\frac{1}{4}\pi\right) + A_2 f\left(\frac{1}{4}\pi\right) + A_3 f\left(\frac{3}{4}\pi\right)$$

that is exact when f is a polynomial of degree 3.

7.2 Numerical Integration Based on Interpolation

- Newton Cotes – general integration formula*

Solution : A polynomial of degree 3 is a linear combination of the four monomials 1, x, x^2, and x^3. Thus, we can determine the coefficients by substituting $f(x) = x^j$ $(0 \le j \le 3)$ and solving the resulting four linear equations. By symmetry, $A_0 = A_3$ and $A_1 = A_2$.

$$0 = \int_{-\pi}^{\pi} 1 \cos x dx = 2A_0 + 2A_1$$

$$-4\pi = \int_{-\pi}^{\pi} x^2 \cos x dx = 2A_0\left(\frac{3}{4}\pi\right)^2 + 2A_1\left(\frac{1}{4}\pi\right)^2$$

The solution is $A_1 = A_2 = -A_0 = -A_3 = \dfrac{4}{\pi}$, and the formula is

$$\int_{-\pi}^{\pi} f(x)\cos dx \approx \frac{4}{\pi}\left[-f\left(-\frac{3}{4}\pi\right) + f\left(-\frac{1}{4}\pi\right) + f\left(\frac{1}{4}\pi\right) - f\left(\frac{3}{4}\pi\right)\right]$$

7.2 Numerical Integration Based on Interpolation

- Newton Cotes*

Example 5 Using the composite Trapezoidal rule and composite Simpson rule to approximate

$$I=\int_0^1 e^{-x}dx,$$

estimate the value of n when a result is required to be correct to 4 singnificance.

Solution : since $0\le x\le 1$, $0.3\le e^{-1}\le e^{-x}\le 1$

Therefore $$0.3<\int_0^1 e^{-x}dx<1$$

If the result is correct to 4 significance, the truncation error should be less than $\frac{1}{2}\times 10^{-4}$.

7.2 Numerical Integration Based on Interpolation

- Newton Cotes*

$$R = -\frac{1}{12}(b-a)h^2 f''(\xi) \quad (8)$$

Since $|f^{(k)}(x)| = e^{-x} \le 1, \quad x \in [0, \ 1],$ by (8)

$$|R_T| = \frac{1}{12}h^2 |f''(\xi)| \le \frac{1}{12}h^2 \le \frac{1}{2}\times 10^{-4}$$

$$R = -\frac{1}{180}(b-a)h^4 f^{(4)}(\xi) \quad (13)$$

i.e. $$n^2 = (\frac{1}{h})^2 \ge \frac{1}{6}\times 10^4 \to n \ge 40.8$$

So n should be 41. By the composite Simpson formula (13)

$$|R_S| = \frac{1}{180}h^4 |f^{(4)}(\xi)| \le \frac{1}{180}h^4 \le \frac{1}{2}\times 10^{-4}$$

therefore $n \ge 3.2$. So n should be 4.

The results indicates that the Composite Simpson's formula has better precision and less computation.

Exercises

$Ex1.$ 1.Validate the trapezoid rule has degree of precision one and the Simpson rule has degree of precision three.

$Ex2.$ 1.Consider the following table of data

x	1.1	1.3	1.5
e^x	3.0042	3.6693	4.4817

Use Simpson rule and composite trapezoid rule to approximate integral.