$MNS\ Computational\ Mathematics\ II/III\ A\ (067021)$

Numerical Analysis 9

Composite rules

If we integrate the piecewise linear polynomial interpolating f at x_i and x_{i+1} where $x_i = a + ih$, h = (b - a)/n and let $f_i = f(x_i)$ then if f, f', f'' are continuous on [a, b]

$$\int_a^b f(x) dx - \frac{h}{2} (f_0 + 2f_1 + \dots + 2f_{n-1} + f_n) = \int_a^b f(x) dx - T(h) = -\frac{h^2(b-a)}{12} f''(\eta)$$

which is the Trapezoidal rule.

Similarly, defining $x_i = a + ih$, where h = (b - a)/(2n), and integrating the piecewise quadratic polynomial we arrive at Simpson's rule

$$\int_a^b f(x) dx = \frac{h}{3} \left(f_0 + 4f_1 + 2f_2 + 4f_3 + \dots + 4f_{2n-3} + 2f_{2n-2} + 4f_{2n-1} + f_{2n} \right) =: S(h).$$

For which the global truncation error is

$$\int_a^b f(x) \mathrm{d} x - S(h) = -\frac{h^4(b-a)}{180} f^4(\eta) \qquad \eta \in (a,b).$$

The Euler-Maclaurin formula is

$$\int_a^b f(x) dx - T(h) = -\frac{1}{12} h^2 \left[f'(b) - f'(a) \right] + \frac{1}{720} h^4 \left[f^{(3)}(b) - f^{(3)}(a) \right] + \cdots$$

Notice that the trapezium rule will be particularly successful for integrands with periodic derivatives.

The method of undetermined coefficients

Make the integration formula exact for polynomials with degree as large as possible.

Formulae using derivatives

Suppose $x_i \in [a, b]$, $f(x_i)$ and $f'(x_i)$ $(i = 1 \to n)$ are given. Assuming that $f, f', \dots, f^{(2n)} \in C[a, b]$, multiplying the Hermite formula by $\omega(x)$ and integrating over [a, b] yields

$$\int_{a}^{b} \omega(x) f(x) dx = \sum_{i=1}^{n} \left\{ H_{i} f(x_{i}) + \overline{H}_{i} f'(x_{i}) \right\} + E_{n}[f] \quad \text{where}$$

$$H_i = \int_a^b \omega(x) h_i(x) \mathrm{d}x, \quad \overline{H}_i = \int_a^b \omega(x) \overline{h}_i(x) \mathrm{d}x, \quad E_n[f] = \frac{1}{(2n)!} \int_a^b \omega(x) \left[w_n(x) \right]^2 f^{(2n)}(\xi) \mathrm{d}x$$

and $w_n(x) = (x - x_1) \cdots (x - x_n)$. Notice that the *n* point Hermite interpolation formula is exact degree for polynomials of degree 2n - 1.

1.F. Blowey

Gaussian Integration

A Gaussian integration formula is one of the form

$$\int_{a}^{b} \omega(x) f(x) dx \approx \sum_{i=1}^{n} H_{i} f(x_{i})$$

where the degree of precision is as large as possible, i.e. at least 2n-1. A sufficient condition is that the x_i 's in the Hermite interpolation formula be chosen so that $\overline{H}_i = 0$.

$$\overline{H}_i = \int_a^b \omega(x) \overline{h}_i(x) \mathrm{d}x = \int_a^b \omega(x) (x-x_i) l_i^2(x) \mathrm{d}x = \int_a^b \omega(x) \frac{w_n(x) l_i(x)}{w_n'(x_i)} \mathrm{d}x.$$

Thus $\overline{H}_i = 0$ if and only if w_n is orthogonal to all polynomials of degree $\leq n - 1$.

Romberg Integration

Suppose $R_{1,1},\cdots,R_{n,1}$ are results obtained from the composite trapezoidal rule with steps $h,\cdots,h/2^n$ where h=(b-a) then applying

$$R_{k,j} = \frac{4^{j-1}R_{k,j-1} - R_{k-1,j-1}}{4^{j-1} - 1}$$

estimates successive terms in the error expansion of the Euler-Macluarin formula.

It is interesting to note that $R_{k,2}$ are the values from Simpson's rule.

Infinite regions and singular integrands

Methods for integrals with an infinite interval:

- Use a Gauss formula;
- Use a change of the variable for the integration such that the infinite interval gets converted to a finite one;
- Use a standard integration formula on an integral with a finite interval and combine
 this with a bound on the remainder.

Methods for integrals where the integrand is singular

- Use a suitable change of variable to remove the singularity;
- Subtract the singular part of the integrand;
- Approximate the integrand by a Taylor series.