Chapter 4 Numerical Differentiation and Integration

Adaptive Quadrature

Quoted from【1】:

Suppose that we wish to approximate $\int_a^b f(x)dx$ to within a specified tolerance $\varepsilon > 0$. The first step in the procedure is to apply Simpson's rule with step size $h = (b-a)/2$. This results in the following.

$$\int_a^b f(x)dx = S(a,b) - \frac{h^5}{90} f^{(4)}(\mu), \text{ for some } \mu \text{ in } (a,b)$$

where

$$S(a,b) = \frac{h}{3}[f(a) + 4f(a+h) + f(b)].$$

The next step is to determine a way to estimate the accuracy of our approximation, in particular, one that does not require determining $f^{(4)}(\mu)$. To accomplish this, we first apply the Composite Simpson's rule with $n = 4$ and step size $(b-a)/4 = h/2$. Thus,

$$\int_a^b f(x)dx = \frac{h}{6}\left[f(a) + 4f\left(a + \frac{h}{2}\right) + 2f(a+h) + 4f\left(a + \frac{3h}{2}\right) + f(b) \right] - \left(\frac{h}{2}\right)^4 \frac{(b-a)}{180} f^{(4)}(\tilde{\mu}),$$

for some $\tilde{\mu}$ in (a,b). To simplify notation, let

$$S\left(a,\frac{a+b}{2}\right)=\frac{h}{6}\left[f(a)+4f\left(a+\frac{h}{2}\right)+f(a+h)\right]$$

and $$S\left(\frac{a+b}{2},b\right)=\frac{h}{6}\left[f(a+h)+4f\left(a+\frac{3h}{2}\right)+f(b)\right].$$

Then Eq. (1) can be rewritten as

$$\int_a^b f(x)dx = S\left(a,\frac{a+b}{2}\right)+S\left(\frac{a+b}{2},b\right)-\frac{1}{6}\left(\frac{h^5}{90}\right)f^{(4)}(\tilde{\mu}).$$

The error estimation is derived by assuming that $\mu \approx \tilde{\mu}$ or, more

precisely that $f^{(4)}(\mu) \approx f^{(4)}(\tilde{\mu})$. The success of the technique

depends on the accuracy of this assumption. If it is accurate, then equating the integrals in Eqs. (1) and (2) implied that

$$S\left(a,\frac{a+b}{2}\right)+S\left(\frac{a+b}{2},b\right)-\frac{1}{16}\left(\frac{h^5}{90}\right)f^{(4)}(\mu)\approx S(a,b)-\frac{h^5}{90}f^{(4)}(\mu),$$

so $$\frac{h^5}{90}f^{(4)}(\mu)\approx\frac{16}{15}\left[S(a,b)-S\left((a,\frac{a+b}{2}\right)-S\left(\frac{a+b}{2},b\right)\right].$$

Using this estimate in Eq. (2) produces the error estimation

$$\left|\int_a^b f(x)dx - S\left(a,\frac{a+b}{2}\right)-S\left(\frac{a+b}{2},b\right)\right|\approx$$

$$\frac{1}{15}\left|S(a,b)-S\left(a,\frac{a+b}{2}\right)-S\left(\frac{a+b}{2},b\right)\right|.$$

This implies that $S(a,(a+b)/2)+S((a+b)/2,b)$ approximates

$\int_a^b f(x)dx$ 15 times better than it agrees with the known value $S(a,b)$.

Thus, if

$$\left| S(a,b) - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right) \right| < 15\varepsilon.$$

then

$$\left| \int_a^b f(x)dx - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right) \right| < \varepsilon.$$

In this case,

$S\left(a, \frac{a+b}{2}\right) + S\left(\frac{a+b}{2}, b\right)$ is assumed to be a sufficiently accurate approximation to $\int_a^b f(x)dx$. Otherwise repeat this procedure until the tolerance is satisfied.

References:

【1】 R. L. Burden and J. D. Faires, *Numerical Analysis*, PWS, Boston, 1993.