

Computer Science/Mathematics 455
Lecture Notes
Lecture # 27

Numerical Integration – Composite Formulas

Need to compute

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

where $f(x)$ has no known antiderivative.

Simple approach — integrate the interpolation polynomial. Let $p_n(x)$ interpolate f at x_0, x_1, \dots, x_n where

$$a \leq x_0 < x_1 < \dots < x_n = b.$$

If $x_k, k = 0, \dots, n$ are evenly spaced, these lead to the *Newton–Cotes* formulas. Like high order interpolation, high order Newton–Cotes formulas do not necessarily lead to more accurate approximations to the integral.

Thus we move to “composite formulas.” We break up the integral into

$$\int_a^b f(x)dx = \sum_{k=0}^{n-1} \int_{x_k}^{x_{k+1}} f(x)dx$$

and apply the approximation formulas to each of the “smaller” integrals in the sum. Generally, we stick with low degree formulas like the Trapezoid rule or Simpson’s rule.

For simplicity, let

$$h = x_{k+1} - x_k = (b - a)/n, \quad \text{Even spacing.}$$

For the Trapezoid Rule,

$$\int_{x_k}^{x_{k+1}} f(x)dx = \frac{h}{2}[f(x_k) + f(x_{k+1})] - \frac{h^3}{12}f''(\xi_k)$$

for $\xi_k \in (x_k, x_{k+1})$. Then if we let

$$T_0(h) = \frac{h}{2} \sum_{k=0}^{n-1} [f(x_k) + f(x_{k+1})] \tag{1}$$

then

$$\begin{aligned}\int_a^b f(x)dx &= T_0(h) - \frac{h^3}{12} \sum_{k=0}^{n-1} f''(\xi_k) \\ &= T_0(h) - n \frac{h^3}{12} f''(\xi) = T_0(h) - \frac{(b-a)h^2}{12} f''(\xi)\end{aligned}$$

for some $\xi \in (a, b)$. Thus approximation error for the composite Trapezoid rule is $O(h^2)$. More on that later.

The formula (1) can be written

$$\begin{aligned}T_0(h) &= \frac{h}{2} \left[\sum_{k=0}^{n-1} f(x_k) + \sum_{k=0}^{n-1} f(x_{k+1}) \right] \\ &= \frac{h}{2} \left[\sum_{k=0}^{n-1} f(x_k) + \sum_{k=1}^n f(x_k) \right] \\ &= \frac{h}{2} [f(x_0) + f(x_n)] + h \sum_{k=0}^{n-1} f(x_k)\end{aligned}$$

Thus the composite trapezoid rule is just a matter of computing a simple sum. If we halve the interval size, we need to evaluate the function f at the midpoints

$$x_{k+1/2} = [x_k + x_{k+1}]/2.$$

We obtain the formula

$$\begin{aligned}T_0(h/2) &= \frac{h}{4} [f(x_0) + f(x_n)] + \frac{h}{2} \sum_{k=0}^{n-1} f(x_k) + \frac{h}{2} \sum_{k=0}^{n-1} f(x_{k+1/2}) \\ &= \frac{1}{2} T_0(h) + \frac{h}{2} \sum_{k=0}^{n-1} f(x_{k+1/2})\end{aligned}$$

Thus with the same function evaluations for $T_0(h/2)$, we can compute both $T_0(h)$ and $T_0(h/2)$. This can be very useful.

The reason is that $T_0(h)$ has an asymptotic error formula. If $I = \int_a^b f(x)dx$ then assuming a sufficient number of continuous derivatives ($2n + 2$) we have

$$T_0(h) = I + a_2 h^2 + a_4 h^4 + \dots + a_{2n} h^{2n} + O(h^{2n+2}).$$

Likewise, for $h/2$ we have

$$T_0(h/2) = I + a_2 h^2/4 + a_4 h^4/16 + \dots + a_{2n} h^{2n}/4^n + O(h^{2n+2}).$$

If we let

$$T_1(h) = (4T_0(h/2) - T_0(h))/3$$

then

$$T_1(h) = I + a'_4 h^4 + a'_6 h^6 + \cdots + a'_{2n} h^{2n} + O(h^{2n+2}).$$

where

$$a'_4 = -a_4/4, \quad a'_{2k} = -(1 - 1/4^{k-1})a_{2k}/3.$$

Thus all of these coefficients become smaller in magnitude.

$T_1(h)$ is the composite Simpson's rule. There is a formula for it, but this one is easier to use. Next time, we continue this extrapolation process to produce Romberg integration.