Trapezoidal Rule

For a single application of the trapezoidal rule, an estimate of the error in the approximation for the integral $I = \int_a^b f(x)dx$ is given by

$$E_t = -\frac{1}{12} f''(\xi)(b-a)^3,$$

where ξ lies somewhere in the interval $[a,b]$. Note that, unlike the expressions for error we developed for interpolating polynomials, there is no value of $\xi \in [a,b]$ that will make this error estimate exact. It is only an estimate, but it is still quite useful.

Now, suppose we estimate the integral by breaking the interval $[a,b]$ up into n subintervals and applying the trapezoidal rule to each subinterval. In particular, let $a = x_0 < x_1 < \cdots < x_n = b$, and rewrite the integral as

$$I = \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} f(x)dx.$$

Applying the trapezoidal rule to each subinterval, we get

$$\begin{aligned} I &= \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} f(x)dx \\ &= \sum_{i=0}^{n-1} (x_{i+1} - x_i) \frac{f(x_i) + f(x_{i+1})}{2}. \end{aligned}$$

This is the formula for the multiple-application trapezoidal rule with arbitrarily spaced intermediate points. If we make the additional simplification that the intermediate points $\{x_0, x_1, \ldots, x_n\}$ are equally spaced, so that each subinterval has size $h = (b-a)/n$, the formula becomes

$$I = \sum_{i=0}^{n-1} (x_{i+1} - x_i) \frac{f(x_i) + f(x_{i+1})}{2}$$

$$= (b-a) \sum_{i=0}^{n-1} \frac{f(x_i) + f(x_{i+1})}{2n}$$

$$= (b-a) \left[\frac{f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)}{2n} \right].$$

This is the multiple-application trapezoidal rule for equally spaced points. Notice that once again, this formula can be regarded as the product of the length of the interval times an estimate of the average value of the function on the interval.

Applying the error estimate given above to each of the subintervals, we get the following estimate of the error in the integral approximation

$$E_a = -\frac{(b-a)^3}{12n^3} \sum_{i=1}^{n} f''(\xi_i)$$

$$= -\frac{(b-a)^3}{12n^2} \left[\frac{1}{n} \sum_{i=1}^{n} f''(\xi_i) \right]$$

$$= -\frac{(b-a)^3}{12n^2} \bar{f}''$$

$$= -\frac{b-a}{12} h^2 \bar{f}'',$$

where ξ_i represents a point in the subinterval $[x_{i-1}, x_i]$, and

$$\bar{f}'' = \frac{1}{n}\sum_{i=1}^{n} f''(\xi_i)$$

represents an estimate of the average value of the second derivative of the function $f(x)$ on the interval $[a,b]$. Notice that this implies that the rate of decrease in the error is *second-order*. That is, the error in the estimate of the integral using the trapezoidal rule is proportional to h^2 or $/n^2$.

Simpson's Rules

The general method of approximating a function with an interpolating polynomial fit to equally-spaced points and then integrating leads to a whole class of approximate integration formulas that are called *Simpson's rules*. The trapezoidal rule is, in fact, a Simpson's rule, but it is seldom referred to in that way. One of the most important and most commonly used integration formulas is called *Simpson's 1/3 rule*, and it is based on using a second-order function approximation.

To derive the single-application version of Simpson's 1/3 rule, we use the Lagrange interpolating polynomial of degree two. Hence, we need to have values of the function at three points $a = x_0 < x_1 < x_2 = b$, which are equally spaced in the interval $[a,b]$. Letting $h = (b-a)/2$, we get

$$
\begin{aligned}
I &= \int_a^b f(x)dx \\
&\approx \int_a^b f_2(x)dx \\
&= \int_{x_0}^{x_2} \left[\begin{aligned} &\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) \\ &+ \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) \end{aligned} \right] dx \\
&= \int_{x_0}^{x_2} \left[\begin{aligned} &\frac{(x-x_0-h)(x-x_0-2h)}{2h^2} f(x_0) - 2\frac{(x-x_0)(x-x_0-2h)}{2h^2} f(x_1) \\ &+ \frac{(x-x_0)(x-x_0-h)}{2h^2} f(x_2) \end{aligned} \right] dx \\
&= \int_{x_0}^{x_2} \left[\begin{aligned} &\frac{(x-x_0)^2 - 3h(x-x_0) + 2h^2}{2h^2} f(x_0) - 2\frac{(x-x_0)^2 - 2h(x-x_0)}{2h^2} f(x_1) \\ &+ \frac{(x-x_0)^2 - h(x-x_0)}{2h^2} f(x_2) \end{aligned} \right] dx \\
&= \int_{x_0}^{x_2} \left[\begin{aligned} &\frac{(f(x_0) - 2f(x_1) + f(x_2))}{2h^2}(x-x_0)^2 - \frac{(3f(x_0) - 4f(x_1) + f(x_2))}{2h}(x-x_0) \\ &+ f(x_0) \end{aligned} \right] dx \\
&= \frac{8h^3}{3}\frac{(f(x_0) - 2f(x_1) + f(x_2))}{2h^2} - \frac{4h^2}{2}\frac{(3f(x_0) - 4f(x_1) + f(x_2))}{2h} + 2hf(x_0) \\
&= \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] \\
&= (b-a)\frac{f(x_0) + 4f(x_1) + f(x_2)}{6}
\end{aligned}
$$

With some additional effort, it can be shown that a single application of Simpson's 1/3 rule has truncation error given by

$$E_t = -\frac{(b-a)^5}{2880} f^{(4)}(\xi)$$
$$= -\frac{b-a}{180} h^4 f^{(4)}(\xi),$$

where $\xi \in [a,b]$. It is important to note that this error is proportional to h^4 instead of h^3, as one might guess without doing the algebra.

Proceeding as we did for the trapezoidal rule, it is straightforward to show that the multiple-application form of Simpson's 1/3 rule becomes

$$I \approx (b-a)\left[\frac{f(x_0) + 4\sum_{i=1,3,5}^{n-1} f(x_i) + 2\sum_{i=2,4,6}^{n-2} f(x_i) + f(x_n)}{3n}\right].$$

Similarly, the estimate of the truncation error for the multiple-application form of Simpson's 1/3 rule becomes

$$E_a = -\frac{b-a}{180} h^4 \bar{f}^{(4)},$$

where $\bar{f}^{(4)}$ represents the average value of the fourth derivative of $f(x)$ on the interval $[a,b]$. Because the rate of decrease in the truncation error for Simpson's 1/3 rule is *fourth-order* rather than just third-order, it is a method that is particularly attractive. Unfortunately, to apply this rule, not only do you need equally-spaced points, but you also need an odd number of data points. For situations where there are an even number of points, one generally resorts to a single application of *Simpson's 3/8 rule*, which requires four data points and is based on using a third-degree interpolating polynomial. The formula for a single application of Simpson's 3/8 rule is given by

$$I \approx (b-a)\frac{f(x_0)+3f(x_1)+3f(x_2)+f(x_3)}{8}.$$

The error estimate for a single application of this rule is given by

$$E_t = -\frac{b-a}{80}h^4 f^{(4)}(\xi),$$

where $h = (b-a)/3$.