INTEGRATION

We wish to integrate a function $f(x)$ within an interval $[a, b]$. Let $m \triangleq (a + b) / 2$; $D \triangleq b - a$; $d \triangleq (b - a) / 2$. Then we can expand the function around the midpoint $m$ in a Taylor series:

$$
 f(x) = f(m) + (x - m)f'(m) + \frac{1}{2} (x - m)^2 f''(m) + \frac{1}{6} (x - m)^3 f'''(m)
 + \frac{1}{24} (x - m)^4 f^{iv}(m) + \frac{1}{120} (x - m)^5 f^{v}(m) + O(x - m)^6. 
$$

(1)

We use this expansion in several ways. First we plug it into the true integral and integrate term by term:

$$
 I \triangleq \int_a^b f(x)dx = \int_a^b \left[ f(m) + (x - m)f'(m) + \frac{1}{2} (x - m)^2 f''(m) + \cdots \right]dx
 = 2df(m) + \frac{1}{3} d^3 f''(m) + \frac{1}{60} d^5 f^{iv}(m) + O(d^7), 
$$

(2)

$$
 = M + E + F + O(d^7),
$$

where the terms with the odd derivatives cancel out. Here $M$ is the Midpoint Rule, one of the standard quadrature rules:

$$
 M \triangleq Df(m) = 2df(m). 
$$

(3)
TRAPEZOIDAL RULE

Next we plug in $a$ and $b$ for $x$ in (1) and add them to get an expansion for the Trapezoidal rule:

$$T \equiv \frac{D}{2} [f(b) + f(a)]$$

$$= 2df(m) + d^3 f''(m) + \frac{1}{12} d^5 f^{iv}(m) + O(d^7), \quad (4)$$

$$= M + 3E + 5F + O(d^7),$$

where again the terms with the odd derivatives cancel out.
LOCAL ERRORS

Equation (2) gives the local truncation error for the Midpoint Rule. The local truncation error for the Trapezoidal Rule is obtained by plugging in equ. (2) in for $M$ in equ. (4):

$$T - I = err_T = 2E + 4F + 6G \cdots$$  \hspace{1cm} (5)

We can also refine the Trapezoidal Rule by splitting the interval $[a, b]$ in two and applying the Trapezoidal Rule to each half, where $m = (a + b)/2$:

$$T_2 = \frac{d}{2} [f(a) + f(m)] + \frac{d}{2} [f(m) + f(b)] = \frac{d}{2} [f(a) + 2f(m) + f(b)]$$  \hspace{1cm} (6)

It is seen that we can write the error for this as follows

$$T_2 - I = err_{T_2} = \frac{1}{2} T + \frac{1}{2} M - I = \frac{1}{2} (T - I) + \frac{1}{2} (M - I)$$

$$= (1E + 2F + 3G + \cdots) - \frac{1}{2} (E + F + G + \cdots)$$  \hspace{1cm} (7)

$$= \frac{1}{2} E + \frac{3}{2} F + \frac{5}{2} G + \cdots$$
EXTRAPOLATION → SIMPSON’S RULE

We can combine the two formulas (5) and (7) above to cancel out the leading terms in the error formulas (5). Let

\[ S \Delta \equiv \frac{4}{3} T_2 - \frac{1}{3} T = \frac{1}{3} d[f(a) + 4f(m) + f(b)] \]

The difference between this expansion and the expansion of the exact integral (2) is the error in \( S \) [note how \( E \) has been cancelled out]:

\[
S - I = err_S = \frac{4}{3} (T_2 - I) - \frac{1}{3} (T - I)
\]

\[ = \frac{2}{3} E + \frac{6}{3} F + \frac{10}{3} G + \cdots - \frac{2}{3} E - \frac{4}{3} F - \frac{6}{3} G - \cdots \]

(8)

\[ = \frac{2}{3} F + \frac{4}{3} G + \cdots = -\frac{1}{90} d^5 f^{iv}(m) + O(d^7). \]
COMPOSITE RULE ERRORS

Divide the interval \([a, b]\) into many little subintervals: (assume each subinterval has the same length \(H\)) \([a, x_1], [x_1, x_2], [x_2, x_3], \ldots, [x_{n-1}, b]\), and apply the trapezoidal rule above to each subinterval. The result is (a closed rule)

\[
T(H) = \frac{1}{2} H \left[ f(a) + 2f(x_1) + \cdots + 2f(x_{n-1}) + f(b) \right].
\]

The composite midpoint rule (an open rule)

\[
M(H) = \frac{1}{2} H \left[ f(x_{1/2}) + 2f(x_{3/2}) + \cdots + 2f(x_{(n-3)/2}) + f(x_{(n-1)/2}) \right].
\]

The Global Truncation Errors for these two rules are just the sums of all the local errors within each subinterval. Using a global estimate for all the local errors (obtained by using an average value for the relevant derivatives), and using the identity \((b - a) = nH\), we get the following for the composite rule errors:

\[
E_T(H) = -\frac{1}{12} (b - a) H^2 f''(\xi) + O(H^4)
\]

\[
E_M(H) = \frac{1}{24} (b - a) H^2 f''(\xi) + O(H^4).
\]

Notice that the powers of \(H\) are even, one less than before. We lose a power of \(H\) because we have \(n = (b - a)/H\) subintervals.
COMPOSITE SIMPSON

Adding up this over many subintervals as above, where $h$ is half the length of each subinterval, we get

$$S(h) = \frac{1}{3} h \left[ f(a) + 4 f(x_{1/2}) + 2 f(x_1) + 4 f(x_{3/2}) + \cdots + 2 f(x_{n-1}) + 4 f(x_{n-1/2}) + f(b) \right],$$

and the global error is (using $b - a = 2nh$):

$$E_{S(h)} = - \frac{1}{180} (b - a) h^4 f^{iv}(\xi) + O(h^6).$$
ROMBERG = GLOBAL EXTRAPOLATION

Simpson’s Rule $S(h)$ can be extrapolated directly from the trapezoidal rule $T(H)$ by combining it with the trapezoidal rule with half the step size: $T(h)$. Since the error in $T(h)$ is $O(h^2)$, we would expect that the error in $T(H)$ would be about $2^2$ times bigger than the error in $T(h)$. Hence we can write

$$ I = T(h) + E_{T(h)} = T(H) + 4E_{T(h)}. $$

Solving for the error $E_{T(h)}$ we get

$$ E_{T(h)} = \frac{1}{3} (T(h) - T(H)). $$

A better approximation to the integral is $T(h) + E_{T(h)}$; if we use our approximation to $E_{T(h)}$ we find that the result is Simpson’s rule:

$$ S = T(h) + E_{T(h)} = \frac{4T(h) - T(H)}{3} $$

Since the error in Simpson’s rule also obeys the $O(h^k)$ law for $k = 4$, we can repeat the same process:

$$ I = S(h) + E_{S(h)} = S(H) + 2^k \cdot E_{S(h)}.$$  

yielding an estimate

$$ E_{S(h)} = \frac{S(h) - S(H)}{2^{2k}}. $$

We can use this to repeat the process, getting the following tableau:

<table>
<thead>
<tr>
<th></th>
<th>$T(H)$</th>
<th>$T(h)$</th>
<th>$S(h)$</th>
<th>$T(h/2)$</th>
<th>$S(h/2)$</th>
<th>$R(h/2)$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$T(h/4)$</td>
<td>$S(h/4)$</td>
<td>$R(h/4)$</td>
<td>$Q(h/4)$</td>
<td>$T(h/8)$</td>
<td>$S(h/8)$</td>
</tr>
</tbody>
</table>
ADAPTIVE = LOCAL EXTRAPOLATION

Consider the single interval Simpson’s rule, over the interval \([a, b]\) with \(2d = D = b - a\). We can compare two Simpson’s rules:

\[
S(d) = \frac{1}{3} d \left[ f(a) + 4 f(m) + f(b) \right]
\]

\[
S(d/2) = \frac{1}{6} d \left[ f(a) + 4 f\left(\frac{a + m}{2}\right) + 2 f(m) + 4 f\left(\frac{m + b}{2}\right) + f(b) \right]
\]

The errors in these two approximations should be related by

\[
E_{S(d)} \approx E_{S(d/2)} \cdot 16
\]

so that we can get an estimate in the error

\[
E_{S(d/2)} \approx \frac{1}{15} \cdot [S(d/2) - S(d)]
\]

just like in Romberg. If this error is too big, split the interval \([a, b]\) into \([a, m]\) and \([m, b]\) and repeat the above on each subinterval. The total integral is approximately the sum of the estimates from the two pieces, and the error in that answer is approximately the sum of the error estimates from each of the two pieces. Each subinterval may be further subdivided recursively. If the total error tolerance desired is \(\text{tol}\), then the error tolerance should be allocated proportionally to each subinterval:

\[
\text{want: } E_{S(d/2)} \leq \text{tol} \cdot \frac{\text{length of subinterval}}{\text{length of whole original interval}} = \text{tol} \cdot [\text{a power of } 2].
\]
In the recursive call, we re-use the values: $f(a)$, $f\left(\frac{a+m}{2}\right)$, $f(m)$, $f\left(\frac{m+b}{2}\right)$, $f(b)$, to make a very efficient method.