The idea utilized here is to take two integral approximations and combine them in a smart way that yields a new approximation that is more accurate. This process in general is called Richardson's extrapolation.

Consider two applications of the composite trapezoidal rule, one with with step size h_1 and another with step size $h_2 < h_1$. The integral $I = \int_a^b f(x)\,dx$ is give by

$$I = I_T(h_1) + E(h_1) = I_T(h_2) + E(h_2) \tag{1}$$

where $I_T(h_i)$ refers to a trapezoidal rule result with step size h_i and errors given by

$$E(h_i) = \frac{b-a}{12} h_i^2 f^{(2)}(c_i)$$

If we assume that $f^{(2)}(c_1) \sim f^{(2)}(c_2) = K =$ constant, then we have

$$\frac{E(h_1)}{E(h_2)} \sim \left(\frac{h_1}{h_2}\right)^2 \longrightarrow E(h_1) \sim \left(\frac{h_1}{h_2}\right)^2 E(h_2)$$

Substituting this back into Eq. (1), we can say:

$$I \sim I_T(h_1) + \left(\frac{h_1}{h_2}\right)^2 E(h_2) = I_T(h_2) + E(h_2)$$

Solve for $E(h_2)$:

$$E(h_2) \sim \frac{I_T(h_1) - I_T(h_2)}{1 - (h_1/h_2)^2}$$

Substitute this back into Eq. (1)

$$\begin{aligned}
I &= I_T(h_2) + E(h_2) \\
&\sim I_T(h_2) + \frac{I_T(h_1) - I_T(h_2)}{1 - (h_1/h_2)^2} \\
&\sim I_T(h_2)\left(\frac{(h_1/h_2)^2}{(h_1/h_2)^2 - 1}\right) - I_T(h_1)\left(\frac{1}{(h_1/h_2)^2 - 1}\right)
\end{aligned}$$

So from two approximations to I, we have constructed a third approximation.

If we double the number of partitions in our second Trapezoidal rule, we would have $h_2 = h_1/2$, and the result simplifies to

$$\begin{aligned}
I &\sim I_T(h_2) + \frac{I_T(h_2) - I_T(h_1)}{3} \\
&\sim \frac{4}{3} I_T(h_2) - \frac{1}{3} I_T(h_1)
\end{aligned}$$

This new estimate has an error $O(h^4)$.

Romberg Table

We can structure the process in a Romberg table in the following manner.

$$
\begin{array}{l|llll}
R_{11} = T_1 & & & & \\
R_{21} = T_2 & R_{22} & & & \\
R_{31} = T_4 & R_{32} & R_{33} & & \\
R_{41} = T_8 & R_{42} & R_{43} & R_{44} & \\
R_{51} = T_{16} & R_{52} & R_{53} & R_{54} & R_{55}
\end{array}
$$

where the first column is initialized using trapezoidal rule where the number of partitions is doubled each time, and the table is filled in using the recursion relations:

$$
\begin{aligned}
R_{k1} &= T_{2^{k-1}} \\
R_{k2} &= R_{k1} + \frac{R_{k1} - R_{k-1,1}}{3} \\
R_{kj} &= R_{k,j-1} + \frac{R_{k,j-1} - R_{k-1,j-1}}{4^{j-1} - 1} \quad k = 2, 3, \ldots, n \quad j = 2, 3, \ldots, k
\end{aligned}
$$

Romberg integration is typically better than Simpson's rule.

Adaptive Quadrature

Question: Can we improve an integration method by having unequally spaced nodes? This could be useful if the integrand is smoothly varying over part of the integration region, and wildly varying over another. To get accuracy in the wildly varying region would put more nodes than needed in the smoothly varying region.

To compute the integral $\int_a^b f(x)\,dx$ to a tolerance of ϵ, we can do the following.

$$\int_a^b f(x)\,dx = S(a,b) + E(a,b)$$

The notation $S(a,b)$ is the integration formula applied to the interval (a,b) (in all cases $c \in [a,b]$ and $h = b - a$):

$$
\begin{aligned}
\text{Trapezoidal rule: } S(a,b) &= \frac{h}{2}(f(a) + f(b)) \text{ and } E(a,b) = -\frac{h^3}{12} f^{(2)}(c) \\
\text{Simpson's rule: } S(a,b) &= \frac{h}{3}(f(a) + 4f(a+h) + f(b)) \text{ and } E(a,b) = -\frac{h^5}{90} f^{(4)}(c)
\end{aligned}
$$

Trapezoidal

Start with, where $c_0 \in [a,b]$:

$$\int_a^b f(x)\,dx = S(a,b) - \frac{h^3}{12} f^{(2)}(c_0) \tag{2}$$

The next step is to halve the region, which will halve the step size, $c_1 \in [a, (a+b)/2]$ and $c_2 \in [(a+b)/2, b]$:

$$
\begin{aligned}
\int_a^b f(x)\,dx &= S(a, \frac{a+b}{2}) + S(\frac{a+b}{2}, b) - \frac{(h/2)^3}{12} f^{(2)}(c_1) - \frac{(h/2)^3}{12} f^{(2)}(c_2) && (3) \\
&= S(a, \frac{a+b}{2}) + S(\frac{a+b}{2}, b) - \frac{1}{4} \cdot \frac{h^3}{12} f^{(2)}(c_3) \text{ where } c_3 \in [a,b] && (4)
\end{aligned}
$$

where in the last step we used the generalized intermediate value theorem. If $f^{(2)}(c_0) \sim f^{(2)}(c_3)$ then we can say Eq. (2) $\sim$ (4), and we have

$$S(a,b) - \frac{h^3}{12}f^{(2)}(c_0) = S(a,\frac{a+b}{2}) + S(\frac{a+b}{2},b) - \frac{1}{4}\cdot\frac{h^3}{12}f^{(2)}(c_0)$$
$$\frac{h^3}{12}f^{(2)}(c_0) = \frac{4}{3}\left(S(a,b) - S(a,\frac{a+b}{2}) - S(\frac{a+b}{2},b)\right)$$

Therefore, using this in Eq. (4), we can say

$$\begin{aligned}\left|\int_a^b f(x)\,dx - S(a,\frac{a+b}{2}) - S(\frac{a+b}{2},b)\right| &\sim \frac{1}{4}\left|\frac{h^3}{12}f^{(2)}(c_2)\right| \\ &\sim \frac{1}{3}\left|S(a,b) - S(a,\frac{a+b}{2}) - S(\frac{a+b}{2},b)\right|\end{aligned}$$

What does this mean? This means that the quantity $S(a,\frac{a+b}{2}) + S(\frac{a+b}{2},b)$ approximates the integral $\int_a^b f(x)\,dx$ about three times better than it approximates $S(a,b)$.

Therefore, if

$$\left|S(a,b) - S(a,\frac{a+b}{2}) - S(\frac{a+b}{2},b)\right| < 3\epsilon$$

we would expect

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

and we could say we have a sufficiently accurate approximation to the integral.

Simpson's rule

Start with, where $c_0 \in [a,b]$:

$$\int_a^b f(x)\,dx = S(a,b) - \frac{h^5}{90}f^{(4)}(c_0) \tag{5}$$

The next step is to halve the region, which will halve the step size, $c_1 \in [a,(a+b)/2]$ and $c_2 \in [(a+b)/2,b]$:

$$\int_a^b f(x)\,dx = S(a,\frac{a+b}{2}) + S(\frac{a+b}{2},b) - \frac{(h/2)^5}{90}f^{(4)}(c_1) - \frac{(h/2)^5}{90}f^{(4)}(c_2) \tag{6}$$
$$= S(a,\frac{a+b}{2}) + S(\frac{a+b}{2},b) - \frac{1}{16}\cdot\frac{h^5}{90}f^{(4)}(c_3) \text{ where } c_3 \in [a,b] \tag{7}$$

where in the last step we used the generalized intermediate value theorem. If $f^{(4)}(c_0) \sim f^{(4)}(c_3)$ then we can say Eq. (5) $\sim$ (7), and we have

$$S(a,b) - \frac{h^5}{90}f^{(4)}(c_0) = S(a,\frac{a+b}{2}) + S(\frac{a+b}{2},b) - \frac{1}{16}\cdot\frac{h^5}{90}f^{(4)}(c_0)$$
$$\frac{h^5}{90}f^{(4)}(c_0) = \frac{16}{15}\left(S(a,b) - S(a,\frac{a+b}{2}) - S(\frac{a+b}{2},b)\right)$$

Therefore, using this in Eq. (7), we can say

$$\left|\int_a^b f(x)\,dx - S(a,\frac{a+b}{2}) - S(\frac{a+b}{2},b)\right| \sim \frac{1}{16}\left|\frac{h^5}{90}f^{(4)}(c_2)\right|$$
$$\sim \frac{1}{15}\left|S(a,b) - S(a,\frac{a+b}{2}) - S(\frac{a+b}{2},b)\right|$$

Therefore, the quantity $S(a,\frac{a+b}{2}) + S(\frac{a+b}{2},b)$ approximates the integral $\int_a^b f(x)\,dx$ about fifteen times better than it approximates $S(a,b)$.

Therefore, if

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

we would expect

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

and we could say we have a sufficiently accurate approximation to the integral.

The process to implement adaptive integration is to subdivide the intervals whenever the error is greater than 15ϵ, until the error inside a subdivision is less than $\epsilon/2^k$ where k is the number of subdivisions that have taken place.

Notes:

- Adaptive Quadrature using Simpson's rule arrives at 15ϵ rather than 3ϵ as the condition for achieving a tolerance of ϵ in the integral.
- Adaptive quadrature typically uses Simpson's rule, although you can set it up for any rule you like.
- In practice, we do choose the factor of 15 to be slightly smaller to allow for the fact that $f^{(4)}(c_0) \sim f^{(4)}(c_3)$ is only an approximation. If the fourth derivative was known to be wildly varying, then we should lower the bound even further.