Adaptive Quadrature

The straightforward application of a composite numerical integration rule such as Simpson’s with the standard upper bound of the error can be much too conservative since the magnitude of the fourth derivative can be large over only a small portion of the interval.

**General Idea:** find an numerical estimate of the integration error so we can decide to accept the estimate to within a fixed tolerance $\epsilon$.

1. Compute the approximation $I_0$ to $\int_a^b f(x)\,dx$;
2. Split the integration interval $[a, b]$ into halves: $[a, c]$ and $[c, b]$.
3. Compute the approximations $I_1$ and $I_2$ over the intervals $[a, c]$ and $[c, b]$.
4. Compare the sum $I_1 + I_2$ with $I_0$ to estimate the error in $I_1 + I_2$.
5. If the estimated error is less than $\epsilon$, accept $I_1 + I_2$ as an approximation to $\int_a^b f(x)\,dx$; otherwise, repeat this process over $[a, c]$ and $[c, b]$ with tolerance $\epsilon/2$.

Now for the details for Simpson’s rule.

For the sake of notation, we shall write $S(\alpha, \beta)$ for the Simpson rule approximation to the integral $\int_\alpha^\beta f(x)\,dx$.

In particular, we shall write:

$$\int_a^b f(x)\,dx = S(a, b) + c_1 h^4 + O(h^6)$$  \hspace{1cm} (1)

Next, subdivide $[a, b]$ and use Simpson’s rule on each half:

$$\int_a^b f(x)\,dx = S(a, c) + S(c, b) + c_1(\frac{h}{2})^4 + O(h^6).$$ \hspace{1cm} (2)

The dominant term in equation (2) is $c_1(\frac{h}{2})^4$ which can be estimated through the identity:

$$S(a, b) + c_1 h^4 + O(h^6) = S(a, c) + S(c, b) + c_1(\frac{h}{2})^4 + O(h^6)$$ \hspace{1cm} (3)

$$0 = [S(a, c) + S(\alpha, b) - S(a, b)] + c_1(\frac{h}{2})^4 - c_1 h^4 + O(h^6)$$ \hspace{1cm} (4)

$$16c_1(\frac{h}{2})^4 - c_1(\frac{h}{2})^4 = S(a, c) + S(a, b) - S(a, b) + O(h^6).$$ \hspace{1cm} (5)

Hence, we take as an estimate of the error term:

$$c_1(\frac{h}{2})^4 \simeq \frac{1}{15} [S(a, c) + S(c, b) - S(a, b)].$$

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Conclude that we will accept the inequality \[
\left| \int_a^b f(x) \, dx - S(a, c) - S(c, b) \right| < \frac{1}{15} |S(a, c) + S(c, b) - S(a, b)| < \frac{\epsilon}{15}.
\]
Note: this reasoning works for any fourth-order rule such as 2-point Gaussian quadrature. Further, if the rule \( Q \) has order \( p \), then the error test is
\[
\frac{1}{2^p - 1} |Q(a, c) + Q(c, b) - Q(a, b)| < \epsilon.
\]
For the sake of completeness, I shall present another strategy.

1. Compute the approximation to \( I_0 \) to \( \int_a^b f(x) \, dx \).
2. Compute another approximation \( I_1 \) to the same integral using a higher order method.
3. Use \( |I_1 - I_0| \) as an error estimate to accept \( I_1 \).

Why is this reasonable?
We start with the approximations and their error estimates:

\[
\int_a^b f(x) \, dx = I_0 + c_0 h^p + o(h^p), \quad (6)
\]
\[
\int_a^b f(x) \, dx = I_1 + c_1 h^q + o(h^q), \quad q > p. \quad (7)
\]
Hence,
\[
0 = I_1 - I_0 + c_0 h^p - c_1 h^q + o(h^p) + o(h^q).
\]
Since \( q > p \), we find
\[
c_0 h^p = I_1 - I_0 + o(h^p).
\]
We conclude that \( I_0 \) is within \( \epsilon \) of \( \int_a^b f(x) \, dx \) if \( |I_1 - I_0| < \epsilon \).