Numerical integration cont.

Use of the error term: For any simple quadrature rule $Q(f)$ of order $r$, we have

\begin{equation}
\int_a^b f(x) \, dx = Q(f) + \text{const}(b-a)^{r+1} f^{(r)}(a \ldots b),
\end{equation}

with $f^{(r)}(a \ldots b)$ denoting some number from the interval

\[ f^{(r)}(a \ldots b) := \left[ \min_{a \leq \eta \leq b} f^{(r)}(\eta) \ldots \max_{a \leq \eta \leq b} f^{(r)}(\eta) \right]. \]

So, if we can determine this interval, then we know that the number $\int_a^b f(x) \, dx$ must lie in the interval $Q(f) + \text{const}(b-a)^{r+1} f^{(r)}(a \ldots b)$.

However, it may be even harder to obtain this interval precisely than it is to evaluate the integral. So, one usually is content with getting some bound $M$ for which

\[ \max_{a \leq \eta \leq b} |f^{(r)}(\eta)| \leq M, \]

which then gives the much cruder error bound

\[ |\int_a^b f(x) \, dx - Q(f)| \leq |\text{const}||b-a|^{r+1}M. \]

Things are more interesting for composite rules. The composite rule $Q_n(f)$ using the simple rule $Q$ of order $r$ on $n$ equal subintervals of $[a \ldots b]$ has the error term

\begin{equation}
\int_a^b f(x) \, dx = Q_n(f) + \text{const}(b-a) \left( \frac{b-a}{n} \right)^r f^{(r)}(a \ldots b),
\end{equation}

with const the same error constant as in the error for the simple rule $Q$. This error term is obtained in the following way: With $t_i := a + ih$, $i = 0 : n$ and $h := (b-a)/n$, we apply the simple rule $Q(f) = Q(f,a,b)$ in (1) to each of the intervals $[t_i \ldots t_{i+1}]$ to find

\[ \int_a^b f(x) \, dx = \sum_{i=0}^{n-1} Q(f,t_i,t_{i+1}) + \sum_{i=0}^{n-1} \text{const}h^{r+1} f^{(r)}(t_i \ldots t_{i+1}). \]

After replacing each $f^{(r)}(t_i \ldots t_{i+1})$ by the larger interval $f^{(r)}(a \ldots b)$, all the summands in the second sum become the same and, using the fact that $nh = b - a$, we obtain the error term in the composite rule (2).

But now the error has a parameter we can play with, namely the number $n$. By making $n$ large, we can, in principle, making the error as small as we like. Also, the bigger the order $r$, the faster the error goes to zero as $n$ grows large.
The typical calculation proceeds as follows: With that bound \( M \) on \( |f^{(r)}| \) in hand, and for a prescribed error tolerance \( \text{tol} \), one ‘solves’ the inequality

\[
\text{const}|b - a|^{r+1}M/n^r \leq \text{tol}
\]

for the smallest integer \( n \) that satisfies it, namely, in \texttt{matlab} terms:

\[
n = \text{ceil}((\text{const} \ (b-a)^{(r+1)} \ M)^{(1/r)});
\]

and uses it.

There are two difficulties with this: one may have difficulty even getting a good bound \( M \); and, the error bound for the composite rule used here is too inaccurate since, after all, we obtained it by replacing each \( f^{(r)}(t_i \ldots t_{i+1}) \) by the possibly much larger \( f^{(r)}(a \ldots b) \).

In adaptive quadrature, one tries to choose the partition \( a = t_0 < t_1 < \ldots < t_n = b \) in such a way that the individual error contributions \( (\Delta t_i)^{r+1}f^{(r)}(t_i \ldots t_{i+1}) \) are, roughly of the same size, thus taking small intervals only where \( |f^{(r)}| \) is ‘large’, while getting away with a few large intervals where \( |f^{(r)}| \) is comparatively small. Further, one makes up for not knowing \( f^{(r)} \) all that well by trying to guess the error from two rules of the same order. Here are the details:

Assume that the interval under consideration is so small that \( f^{(r)} \), i.e., \( f^{(r)}(a \ldots b) \) is, essentially, a constant. Then, on abbreviating the terms in (2) as follows:

\[
I = Q_n(f) + E_n,
\]

we conclude that

\[
E_{2n} = \text{const}(b - a)^{r+1}/(2n)^r f^{(r)}(a \ldots b) = E_n/2^r,
\]

i.e.,

\[
Q_n(f) + 2^r E_{2n} = I = Q_{2n}(f) + E_{2n},
\]

which we can solve for \( E_{2n} \) to find

\[
(3) \quad E_{2n} = \frac{Q_{2n}(f) - Q_n(f)}{2^r - 1}.
\]

Now, this may or may not be a good estimate for the error; it all depends on whether the assumption made, namely that \( f^{(r)} \) doesn’t vary much over the interval \([a \ldots b] \), actually holds. For a small enough interval, this will be the case, and then we might as well add this estimate for the error to our approximate value \( Q_{2n}(f) \) for an even better approximation

\[
Q_{2n}(f) + \frac{Q_{2n}(f) - Q_n(f)}{2^r - 1}.
\]

Since this better estimate is based on a certain model of convergence of \( Q_n(f) \) as \( n \to \infty \), this process of getting a better approximation is also called \textbf{extrapolation to the limit}.

The book describes the use of such error estimates in adaptive quadrature quite well. To that description, I want to add that professional quadrature packages use a Gauss rule as the underlying simple rule rather than a NC rule.