Numerical integration cont.

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

$$\int_a^b f(x)\,\mathrm{d}x = Q(f) + \mathrm{const}(b-a)^{r+1} f^{(r)}(a\,..\,b), \tag{1}$$

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

$$f^{(r)}(a\,..\,b) := [\min_{a\le\eta\le b} f^{(r)}(\eta)\,..\,\max_{a\le\eta\le b} f^{(r)}(\eta)].$$

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

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

$$\max_{a\le\eta\le b} |f^{(r)}(\eta)| \le M,$$

which then gives the much cruder error bound

$$|\int_a^b f(x)\,\mathrm{d}x - Q(f)| \le |\mathrm{const}||b-a|^{r+1} M.$$

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 $[a\,..\,b]$ has the error term

$$\int_a^b f(x)\,\mathrm{d}x = Q_n(f) + \mathrm{const}(b-a)\left(\frac{b-a}{n}\right)^r f^{(r)}(a\,..\,b), \tag{2}$$

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 $[t_i\,..\,t_{i+1}]$ to find

$$\int_a^b f(x)\,\mathrm{d}x = \sum_{i=0}^{n-1} Q(f, t_i, t_{i+1}) + \sum_{i=0}^{n-1} \mathrm{const} h^{r+1} f^{(r)}(t_i\,..\,t_{i+1}).$$

After replacing each $f^{(r)}(t_i\,..\,t_{i+1})$ by the larger interval $f^{(r)}(a\,..\,b)$, 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* *tol*, one 'solves' the inequality

$$\text{const}|b-a|^{r+1}M/n^r \le tol$$

for the smallest integer n that satisfies it, namely, in `matlab` terms:

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n = ceil((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 $f^{(r)}(t_i \mathrel{..} t_{i+1})$ by the possibly much larger $f^{(r)}(a \mathrel{..} b)$.

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 $(\Delta t_i)^{r+1} f^{(r)}(t_i \mathrel{..} t_{i+1})$ 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., $f^{(r)}(a \mathrel{..} b)$ is, essentially, a constant. Then, on abbreviating the terms in (2) as follows:

$$I = Q_n(f) + E_n,$$

we conclude that

$$E_{2n} = \text{const}(b-a)^{r+1}/(2n)^r f^{(r)}(a \mathrel{..} b) = E_n/2^r,$$

i.e.,

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

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

$$E_{2n} = \frac{Q_{2n}(f) - Q_n(f)}{2^r - 1}. \tag{3}$$

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 $[a \mathrel{..} b]$, 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 **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.