Adaptive Quadrature

$$f^{(k+1)}(\xi)$$

We know neither $f^{(k+1)}$ nor ξ, so can we actually *use* the truncation error formulas?

Let $I \equiv \int_a^b f(x)dx$, and consider the Simpson's approximation

$$I = S(a,b) + E(a,b) \equiv \frac{h}{3}(f(a) + 4f(\tfrac{a+b}{2}) + f(b)) - \frac{h^5}{90}f^{(4)}(\xi)$$

and the two Simpson's approximations over the halved interval:

$$\begin{aligned} I &= S(a, \tfrac{a+b}{2}) + E(a, \tfrac{a+b}{2}) \quad + \quad S(\tfrac{a+b}{2}, b) + E(\tfrac{a+b}{2}, b) \\ &= S(a, \tfrac{a+b}{2}) + S(\tfrac{a+b}{2}, b) - \tfrac{(h/2)^5}{90} f^{(4)}(\xi_l) - \tfrac{(h/2)^5}{90} f^{(4)}(\xi_r). \end{aligned}$$

Now we make a wish: *assume*

$$f^{(4)}(\xi) \approx f^{(4)}(\xi_l) \approx f^{(4)}(\xi_r) \qquad \text{(wish)}.$$

Then

$$\begin{aligned} I &= S(a,b) - \tfrac{h^5}{90} f^{(4)}(\xi) \\ &\approx S(a, \tfrac{a+b}{2}) + S(\tfrac{a+b}{2}, b) - 2\tfrac{(h/2)^5}{90} f^{(4)}(\xi) \\ &= S(a, \tfrac{a+b}{2}) + S(\tfrac{a+b}{2}, b) - \tfrac{1}{16}\tfrac{h^5}{90} f^{(4)}(\xi) \end{aligned}$$

or

$$E \;\equiv\; S(a, \tfrac{a+b}{2}) + S(\tfrac{a+b}{2}, b) - S(a,b) \;\approx\; \frac{15}{16}E(a,b) \;\approx\; 15(E(a, \tfrac{a+b}{2}) + E(\tfrac{a+b}{2}, b)).$$

This is an error estimate that we have in our hand; *not* an error formula *nor* an upper bound, but a *computed approximation* to the actual error. Methods other than Simpson's method would give analogous results, but with weights different than 15/16 and 1/16. If you are worried about (wish), then you might use 10 in place of 15, but the worry is misguided if the algorithm that we are developing proceeds very many steps.

So what? Well suppose we want to compute an approximation to I with error at most τ. Then if $E \leq 15\tau$ we have reason to believe – modulo (wish) – that our finer approximation $I \approx S(a, \frac{a+b}{2}) + S(\frac{a+b}{2}, b)$ will do.

What if $E > 15\tau$? Set $a_l = a,\ b_l = \frac{a+b}{2} = a_r$, and $b_r = b$, and notice that we can apply the analysis above to each of the integrals $I_l \equiv \int_{a_l}^{b_l} f(x)dx$ and $I_r \equiv \int_{a_r}^{b_r} f(x)dx$. So (taking I_l first), compute $E_l \equiv S(a_l, \frac{a_l+b_l}{2}) + S(\frac{a_l+b_l}{2}, b_l) - S(a_l, b_l)$. If $E_l \leq 15(\tau/2)$, then we take $I_l \approx S_l \equiv S(a_l, \frac{a_l+b_l}{2}) + S(\frac{a_l+b_l}{2}, b_l)$, if not then we split I_l into I_{ll} and I_{lr}, etc... It may take many splittings to achieve the error tolerance (which gets halved at each splitting), but eventually we will satisfy the $E_* < 15(\tau/2^k)$ condition and then we add up our sub-approximations to get an approximation S_l to I_l. When the same is done for I_r we have $I = I_l + I_r \approx S_l + S_r + E_l + E_r$, where – modulo (wish) – $|E_l + E_r| \leq \tau/2 + \tau/2 = \tau$.

All of this discussion can be reduced to a recursive algorithm $R(a, b, \tau)$:

$$\begin{aligned} \text{If } S(a, \tfrac{a+b}{2}) + S(\tfrac{a+b}{2}, b) - S(a,b) < 15\tau: &\quad \text{Set } S = S(a, \tfrac{a+b}{2}) + S(\tfrac{a+b}{2}, b) \text{ and quit.} \\ \text{Else:} &\quad \text{Set } S = R(a, \tfrac{a+b}{2}, \tau/2) + R(\tfrac{a+b}{2}, b, \tau/2). \end{aligned}$$