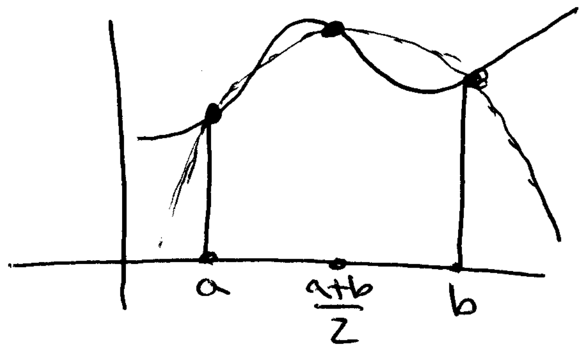
Adaptive Integration

Previously, we have decided on the number of ~~integr~~ steps in numerical integration using an a priori bound on f'', or in the case of the Romberg algorithm, we just rely on the fast convergence of the method (we could derive an explicit error bound, but it would require knowing a long list of derivatives of f at the endpoints).

Suppose we are handed a function and an error bound ϵ. Can we integrate without explict bounds on a derivative?

We will base the method on Simpson's rule.

Idea:



Fit a quadratic to f at $a, \frac{a+b}{2}, b$ and integrate it.

We only need to integrate $1, x,$ and x^2 with a formula like

$$\int_a^b f(x)\,dx \approx A f(a) + B f\left(\frac{a+b}{2}\right) + C f(b)$$

We let $a=-1, b=1$ and observe

$$\int_{-1}^{1} 1\,dx = 2 = A + B + C$$

$$\int_{-1}^{1} x\,dx = 0 = A(-1) + B(0) + C(1)$$

$$\int_{-1}^{1} x^2\,dx = \frac{2}{3} = A(1) + B(0) + C(1).$$

This leaves us with

$$\begin{aligned} 2 &= A+B+C \\ 0 &= -A+C \quad \text{so } C=A \\ \frac{2}{3} &= A+C. \quad C=A=1/3, \end{aligned}$$

$B = 4/3.$

we get

$$\int_{-1}^{1} f(x)\,dx \approx \frac{1}{3}\left[f(-1) + 4f(0) + f(1)\right].$$

Now to transform to $[a,b]$, we let

$$y = \frac{b(x+1)}{2} - \frac{a(x-1)}{2}, \quad \text{so } y(-1)=a, \; y(1)=b.$$

we have

$$dy = \left(\frac{b}{2} - \frac{a}{2} = \frac{(b-a)}{2}\right)dx.$$

Then we have

$$\int_{-1}^{1} f(x)\,dx = \int_a^b f(y)\frac{2}{(b-a)}\,dy$$

$$= \frac{2}{(b-a)}\int_a^b f(y)\,dy.$$

Thus

$$\int_a^b f(y)\,dy \approx \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right].$$

If $b = a+2h$, we have

$$\int_a^{a+2h} f(x)\,dx \approx \frac{h}{3}\left[f(a) + 4f(a+h) + f(a+2h)\right].$$

Now let's derive an error term.

$$\begin{aligned} f(a+h) &= \\ &= f(a) + hf'(a) + \frac{h^2}{2}f''(a) + \frac{h^3}{3!}f'''(a) + \dots \end{aligned}$$

$$f(a+2h) = f(a) + 2hf'(a) + \frac{4h^2}{2}f''(a) + \frac{8h^3}{3!}f'''(a) + \dots$$

so we have

$$\begin{aligned} &f(a) + 4f(a+h) + f(a+2h) = \\ &\quad 6f(a) + 6f'(a)h + 4f''(a)h^2 + 2f'''(a)h^3 \\ &\quad\quad + \left(\frac{1}{3!} + \frac{16}{4!}\right)f''''(a)h^4 + \dots \end{aligned}$$

and

This means that our Simpson's rule approximation is

$$2 f(a)\, h + \cancel{2f'(a)h^2} + \cancel{\tfrac{4}{3} f''(a)\, h^3}$$
$$+ \frac{2}{3} f'''(a)\, h^4 + \frac{20}{3\cdot 4!} f''''(a)\, h^5 + \cdots$$

Now on the other hand, if we let

$$F(x) = \int f(x)\,dx,$$

by ~~term-by-term integration~~ we have

$$F(a+2h) = F(a) + F'(a)(2h) + F''(a)\frac{(2h)^2}{2}$$
$$+ F'''(a)\frac{(2h)^3}{3!} + F''''(a)\frac{(2h)^4}{4!} + F'''''(a)\frac{(2h)^5}{5!}$$
$$= F(a) + \cancel{f(a)\cdot 2h} + \cancel{2f'(a)h^2}$$
$$+ \cancel{\frac{4}{3} f''(a) h^3} + \cancel{\frac{4}{3!} f'''(a) h^4} + \cdots$$
$$+ \frac{32}{5!} f''''(a) h^5 + \cdots$$

Comparing the two series, we have

$$\left(\int_a^{a+2h} f(x)\,dx = F(a+2h)-F(a)\right) - \frac{h}{3}\left[f(a) + 4f(a+h) + f(a+2h)\right]$$

$$= \left(\frac{32}{5!} - \frac{20}{3\cdot 4!}\right) f''''(a)\, h^5 + \cdots$$

$$= \left(\frac{4\cdot 6}{5\cdot 3\cdot 6} - \frac{5\cdot 5}{3\cdot 6\cdot 5}\right) f''''(a)\, h^5 + \cdots$$

$$= -\frac{1}{90} f''''(a)\, h^5 + \cdots$$

It's perhaps not surprising that $\exists$ some ξ between a and $a+2h$ so

$$\text{Error}_{\text{simpson}} = -\frac{1}{90} h^5 f''''(\xi).$$

To apply Simpson's rule over n points, (where n is divisible by 2) we simply compute

$$\frac{h}{3}\left[f(a=x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + \cdots + 4f(x_{n-1}) + f(x_n=b)\right]$$

The error estimate is the sum of $n/2$ of the previous error estimates, or

$$\sum_{i=1}^{n/2} -\frac{1}{90} f''''(\xi_i)\, h^5 = \left(-\frac{1}{90}\right) h^5 \sum_{i=1}^{n/2} f''''(\xi_i)$$

$$= -\frac{1}{90} h^4 \frac{(b-a)}{n} \sum_{i=1}^{n/2} f''''(\xi_i)$$

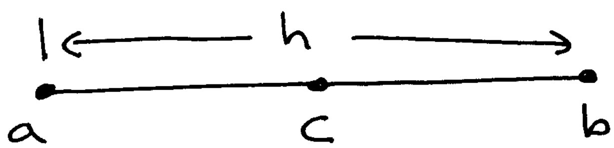
$$= -\frac{1}{90} \frac{h^4 (b-a)}{2} \cdot \boxed{\frac{1}{n/2} \sum_{i=1}^{n/2} f''''(\xi_i)} \leftarrow \text{average at } n/2 \text{ points}$$

$$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \parallel$$

$$= -\frac{1}{180} h^4 (b-a)\, f''''(\xi) \leftarrow \text{value at some point}$$

Next time: adapting to a variable integrand!

We now use this error estimate to study when we should further subdivide an interval in adaptive integration with bound ϵ.



Let $S(a,b) = \dfrac{(b-a)}{6}\left[f(a) + 4f\left(\dfrac{a+b}{2}\right) + f(b) \right]$

and $E(a,b) = -\dfrac{1}{90}\left(\dfrac{b-a}{2}\right)^5 f^{(4)}(a) + \ldots\ldots$

Now $\quad = -\frac{1}{90}\left(\frac{h}{2}\right)^5 f^{(4)}(a) + \ldots$

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

Since these terms come from one application of Simpson's rule, we call them $S^{(1)}$ and $E^{(1)}$.

If we split (a,b) into (a,c), (c,b) and apply Simpson's rule to both parts, we get

$$S^{(2)} = S(a,c) + S(c,b)$$

$$E^{(2)} = -\frac{1}{90}\left(\frac{h/2}{2}\right)^5 f^{(4)}(a) + \dots + -\frac{1}{90}\left(\frac{h/2}{2}\right)^5 f^{(4)}(c) + \dots$$

Now if we assume (falsely!) that the interval is small enough that $f^{(4)}(x) \approx C$ on (a,b), we have

$$E^{(1)} = -\frac{1}{90}\left(\frac{h}{2}\right)^5 C$$

$$E^{(2)} = -\frac{2}{90}\left(\frac{1}{2}\right)^5\left(\frac{h}{2}\right)^5 C = \left(\frac{1}{16}\right)\left(-\frac{1}{90}\left(\frac{h}{2}\right)^5 C\right).$$

or $E^{(1)} = 16\, E^{(2)}$

Now

$$I = S^{(1)} + E^{(1)}$$

$$I = S^{(2)} + E^{(2)}$$

so

$$0 = S^{(2)} - S^{(1)} + E^{(2)} - E^{(1)}$$

or

$$E^{(1)} - E^{(2)} = S^{(2)} - S^{(1)}$$

or

$$15\, E^{(2)} = S^{(2)} - S^{(1)}.$$

Thus

$$I = S^{(2)} + \frac{1}{15}\left(S^{(2)} - S^{(1)}\right)$$

We've now written $E^{(2)}$ (at least approximately) in terms of things we can compute.

Subdivision test. If we can permit error $\epsilon > 0$ on $[a,b]$, then we subdivide if $\frac{1}{15}(S^{(2)} - S^{(1)}) \geq \epsilon$.

Remember, when subdividing, that you should only permit half as much error on the subintervals!