Richardson extrapolation

$$\phi(h) = \frac{f(x+h) - f(x-h)}{2h} = f'(x) + \frac{1}{3!} f'''(x) h^2 + \frac{1}{5!} f^{(5)}(x) h^4 + \underline{\quad\quad} h^6$$

$$\phi\left(\frac{h}{2}\right) = f'(x) + \frac{1}{4} \cdot \frac{1}{3!} f'''(x) h^2 + \frac{1}{16} \cdot \frac{1}{5!} f^{(5)}(x) h^4 + \underline{\quad} h^6$$

$$\tilde{\phi}(h) = \frac{1}{3}\left(4\phi\left(\frac{h}{2}\right) - \phi(h)\right) = f'(x) + \underline{\quad\quad\quad} h^4 + \underline{\quad\quad} h^6$$

(4-th order accuracy)

$$\tilde{\phi}\left(\frac{h}{2}\right) = f'(x) + \frac{1}{16} \cdot \underline{\quad\quad\quad} h^4 + \underline{\quad\quad} h^6 + \cdots$$

$$\frac{1}{15}\left(16\,\tilde{\phi}\left(\frac{h}{2}\right) - \tilde{\phi}(h)\right) = f'(x) + \underline{\quad} h^6 + \cdots$$

(6-th order accuracy)

Generally, if a numerical approximation $\phi(h)$ for a quantity L has error term

$$\phi(h) = L + a_k h^k + \text{higher order terms}$$

then

$$\tilde{\phi}(h) = \frac{1}{2^k - 1}\left(2^k \phi\left(\frac{h}{2}\right) - \phi(h)\right)$$

has higher order accuracy.

This can be applied iteratively.

7.2 Numerical integration (quadrature) based on interpolation

Question : Given $f(x)$ on $[a,b]$, approximate $\int_a^b f(x)\,dx$

- Even if f is given by a formula, $\int_a^b f(x)\,dx$ may not be

Calculated analytically. $\int_0^1 e^{-x^2} dx$

Suppose we utilize pt values at $x_0, x_1, \cdots, x_n$ in $[a,b]$.

$$f(x) = \sum_{i=0}^{n} f(x_i)\, l_i(x) + \frac{1}{(n+1)!} f^{(n+1)}(\xi_x) \prod_{i=0}^{n} (x - x_i)$$

$$l_i(x) = \prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{x - x_j}{x_i - x_j}$$

$$\int_a^b f(x)\,dx = \underbrace{\sum_{i=0}^{n} f(x_i) \int_a^b l_i(x)\,dx}_{\text{approximation}} + \underbrace{\frac{1}{(n+1)!} \int_a^b f^{(n+1)}(\xi_x) \prod_{i=0}^{n} (x - x_i)\,dx}_{\text{error}}.$$

$$|\text{error}| \le \frac{1}{(n+1)!} \max_{x\in[a,b]} \left| f^{(n+1)}(x) \right| \cdot \int_a^b \prod_{i=0}^{n} |x - x_i|\,dx.$$

Case $n=1$, $x_0 = a$, $x_1 = b$

$$l_0(x) = \frac{x - x_1}{x_0 - x_1} = -\frac{x-b}{b-a}$$

$$\int_a^b l_0(x)\,dx = -\frac{1}{b-a} \cdot \frac{1}{2}(x-b)^2 \Big|_a^b = \frac{1}{2}(b-a)$$

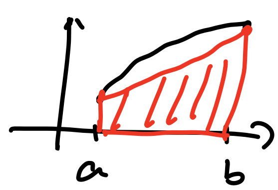
$$l_1(x) = \frac{x - x_0}{x_1 - x_0} = \frac{x-a}{b-a}$$

$$\int_a^b l_1(x)\,dx = \frac{1}{2}(b-a)$$

$$\Rightarrow \int_a^b f(x)\,dx \approx \frac{1}{2}(b-a)\cdot f(a) + \frac{1}{2}(b-a)\cdot f(b)$$

$$= \frac{1}{2}(b-a)\cdot\big(f(a) + f(b)\big)$$

"trapezoid rule"



$$\text{error} \le \frac{1}{2} \max_{x\in[a,b]} |f''(x)| \cdot \underbrace{\int_a^b |(x-a)(x-b)|\,dx}_{\frac{1}{6}(b-a)^3}$$

$$= \frac{1}{12} \max_{x\in[a,b]} |f''(x)| \cdot (b-a)^3$$

Case $n=2,\ x_0 = a,\ x_1 = \frac{a+b}{2},\ x_2 = b$

$h = \frac{b-a}{2}$

$$l_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} = \frac{(x-x_1)(x-x_2)}{2h^2}$$

$$\int_a^b l_0(x)\,dx = \frac{1}{2h^2}\int_a^b (x-(a+h))(x-(a+2h))\,dx$$

$y = x-a$

$$= \frac{1}{2h^2}\int_0^{2h} \underbrace{(y-h)(y-2h)}_{y^2-3hy+2h^2}\,dy$$

$$= \frac{1}{2h^2}\left(\frac{1}{3}y^3 - 3h\cdot\frac{1}{2}y^2 + 2h^2 y\right)\Big|_0^{2h}$$

$$= \frac{1}{2h^2}\cdot h^3\left(\frac{8}{3} - \frac{3}{2}\cdot 4 + 2\cdot 2\right) = \frac{1}{3}h$$

$$\frac{8}{3} - 6 + 4$$

Similarly, $\int_a^b l_1(x)\,dx = \frac{4}{3}h$, $\int_a^b l_2(x)\,dx = \frac{1}{3}h$

$$\Rightarrow \int_a^b f(x)\,dx \approx \frac{1}{3}h\cdot f(x_0) + \frac{4}{3}h\cdot f(x_1) + \frac{1}{3}h\cdot f(x_2)$$

$$= \frac{1}{6}(b-a)\cdot\left(f(x_0) + 4f(x_1) + f(x_2)\right)$$

"Simpson's rule".

$$\text{error} \le \frac{1}{6}\cdot\max_{x\in[a,b]}|f'''(x)|\cdot \underbrace{\int_a^b \left|(x-a)\left(x-\frac{a+b}{2}\right)(x-b)\right|dx}_{\frac{1}{32}(b-a)^4}$$

$$= \frac{1}{192}\max_{x\in[a,b]}|f'''(x)|\cdot(b-a)^4$$

(It's not optimal !)

In fact

$1\cdot \quad f(a) = f(a)$

$4\cdot \quad f(a+h) = f(a) + f'(a)h + \frac{1}{2}f''(a)\cdot h^2 + \frac{1}{6}f'''(a)\cdot h^3 + \frac{1}{24}f^{(4)}(a)\cdot h^4 + \cdots$

$1\cdot \quad f(a+2h) = f(a) + 2f'(a)h + 2f''(a)\cdot h^2 + \frac{4}{3}f'''(a)\cdot h^3 + \frac{2}{3}f^{(4)}(a)\cdot h^4 + \cdots$

$$\text{RHS} = \frac{h}{3}\left(6f(a) + 6f'(a)h + 4f''(a)h^2 + 2f'''(a)h^3 + \frac{5}{6}f^{(4)}(a)h^4 + \cdots\right)$$

$$\text{LHS} = \int_0^{2h} f(a+x)\,dx$$

$$= \int_0^{2h}\left(f(a) + f'(a)x + \frac{1}{2}f''(a)\cdot x^2 + \frac{1}{6}f'''(a)\cdot x^3 + \frac{1}{24}f^{(4)}(a)\cdot x^4 + \cdots\right)dx$$

$$= f(a)\cdot 2h + f'(a)\cdot\frac{1}{2}(2h)^2 + \frac{1}{2}f''(a)\frac{1}{3}(2h)^3 + \frac{1}{6}f'''(a)\cdot\frac{1}{4}(2h)^4 + \frac{1}{24}f^{(4)}(a)\cdot\frac{1}{5}(2h)^5 + \cdots$$

RHS coeff. : $2, 2, \frac{4}{3}, \frac{2}{3}, \frac{5}{18}$

LHS coeff : $2, 2, \frac{4}{3}, \frac{2}{3}, \frac{4}{15}$

$$\text{error} = \underbrace{\left(\frac{4}{15} - \frac{5}{18}\right)}_{-\frac{1}{90}} f^{(4)}(a)\cdot h^5 + \cdots$$

$$|\text{error}| \le \frac{1}{90}\max_{x\in[a,b]}|f^{(4)}(a)|\cdot h^5$$

- The accuracy of a quadrature depends on whether it is exact for low degree polynomials.
- If a quadrature $\int_a^b f(x)\,dx \approx \sum_{i=0}^{n} c_i f(x_i)$ is exact for polynomials w/ $\deg \le k$, then $\text{error} \le O(h^{k+2})$ $\quad h \sim b-a$

$$f(x) = \underbrace{f(a) + f'(a)(x-a) + \cdots + \frac{1}{k!} f^{(k)}(a)(x-a)^k}_{\deg \le k \text{ poly.}} + \underbrace{\frac{1}{(k+1)!} f^{(k+1)}(\xi_x)(x-a)^{k+1}}_{\text{error} \sim O(h^{k+1})}$$

- If a quadrature is derived from poly. interp. w/ $x_0, \cdots, x_n$, then error $\le O(h^{n+2})$ because it is exact for poly. w/ $\deg \le n$. (this may not be optimal)
- Simpson's rule is exact for poly. w/ $\deg \le 3$ (although derived from $n=2$ poly. interp.)

  (check exactness for $(x - \frac{a+b}{2})^3$).