Error estimate $E_n \equiv I - I_n \sim \frac{C}{n^p}$

$p=2$ for trapezoidal rule

$p=4$ for Simpson's rule

Richardson's extrapolation formula

$$I - I_{2n} \sim \frac{C}{(2n)^p} = \frac{1}{2^p} \cdot \frac{C}{n^p} \sim \frac{1}{2^p} \cdot (I - I_n)$$

$$\therefore I \sim \frac{1}{2^p - 1}\left[2^p I_{2n} - I_n\right] \equiv R_{2n}$$

Application:

$$I_{2n} - I_n = (I - I_n) - (I - I_{2n})$$
$$\approx (2^p - 1)(I - I_{2n})$$

$$I_{4n} - I_{2n} = (I - I_{2n}) - (I - I_{4n})$$
$$\sim \left(1 - \frac{1}{2^p}\right) \cdot (I - I_{2n})$$

$$\frac{I_{2n} - I_n}{I_{4n} - I_{2n}} \approx \frac{(2^p - 1)(I - I_{2n})}{\left(1 - \frac{1}{2^p}\right)(I - I_{2n})} = 2^p$$

$$\therefore \quad P = \log\left(\frac{I_{2n} - I_n}{I_{4n} - I_{2n}}\right) / \log 2$$

Application: $I = \int_0^1 \sqrt{x}\, dx$

Simpson's rule for $\sqrt{x}$

n	Error	Ratio $\equiv \frac{I_{3n} - I_{2n}}{I - I_{4n}}$
2	2.860×10^{-2}	
4	1.014×10^{-2}	2.82
8	3.587×10^{-3}	2.83
16	1.268×10^{-3}	2.83
32	4.485×10^{-3}	2.83

$$P = \log(2.82) / \log(2) = 1.50$$

$$\therefore \quad I - I_n \sim \frac{c}{n^{1.5}}$$

Trapezoidal rule for $\sqrt{x}$

n	Error	Ratio
2	6.31×10^{-2}	
4	2.34	2.70
8	8.54×10^{-3}	2.74
16	3.09	2.77
32	1.11	2.79
64	3.96×10^{-4}	2.80
128	1.41	2.81

$P = \log(2.81)/\log(2)$
~ 1.5

The exponent p depends on the method and the function in the integrand.

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(a) $E_n \equiv I - I_n \qquad I \equiv \int_0^1 f(x)\,dx$

For Trapezoidal rule:

$$I_n = \int_0^1 f(0) + (f(1) - f(0))x \quad dx$$

$$E_n = I - I_n$$

$$= \int_0^1 f(x)\,dx - \int_0^1 f(0) + (f(1) - f(0))x\,dx$$

$$= \int_0^1 f(x)\,dx - \frac{f(1) + f(0)}{2}$$

$$\int_0^1 k(t)\, f'(t)\,dt$$

$$= k(t)\, f(t)\Big|_0^1 - \int_0^1 k'(t)\, f(t)\,dt$$

$$k(t) = \frac{t_{j-1} + t_j}{2} - t \qquad k'(t) = -1$$

for the whole domain $k(t) = \frac{1}{2} - t$

$$\therefore \int_0^1 k(t)\, f'(t)\,dt = +\int_0^1 f(t)\,dt - \frac{f(1)+f(0)}{2} = E_n \text{ for Trapezoidal Rule}$$

(b) $f(x) = x^\alpha$

$$E_n = \sum_{j=1}^{n} \int_{t_{j-1}}^{t_j} \left(\frac{t_{j-1}+t_j}{2} - t\right)(\alpha t^{\alpha-1})\, dt$$

$$= \sum_{j=1}^{n} \int_{t_{j-1}}^{t_j} \left(\frac{t_{j-1}+t_j}{2}\alpha t^{\alpha-1} - \alpha t^\alpha\right) dt$$

$$= \sum_{j=1}^{n} \left(\frac{t_{j-1}+t_j}{2}\, t^\alpha \Big|_{t_{j-1}}^{t_j} - \frac{\alpha}{\alpha+1} t^{\alpha+1} \Big|_{t_{j-1}}^{t_j} \right)$$

$t_j = \frac{j}{n}$, $j = 0, 1, \cdots, n$

$$= \sum_{j=1}^{n} \left\{ \frac{2j-1}{2n} \left[\left(\frac{j}{n}\right)^\alpha - \left(\frac{j-1}{n}\right)^\alpha \right] - \frac{\alpha}{\alpha+1}\left[\left(\frac{j}{n}\right)^{\alpha+1} - \left(\frac{j-1}{n}\right)^{\alpha+1} \right] \right\}$$

$$= \frac{1}{n^{1+\alpha}} \sum_{j=1}^{n} \left[\frac{2j-1}{2}\left(j^\alpha - (j-1)^\alpha\right) - \frac{\alpha}{\alpha+1}\left(j^{\alpha+1} - (j-1)^{\alpha+1}\right) \right]$$

more algebra shows that

$$E_n \sim \frac{C}{n^{\alpha+1}} \qquad p = \alpha+1$$

for $\alpha = \frac{1}{2}$, $p = 1.5$ as in the previous example.

Why is $p = 1.5$ lower than the true order $p = 2$?

numerical integration:

$$I_n(f) = \sum_{j=1}^{n} w_j f(x_j)$$

nodes $[x_j]$ & weights $[w_j]$ are chosen so that

$I_n(f) = I(f)$ for all polynomials $f(x)$ of as large a

degree as possible.

$\Rightarrow$ Theorem 5.3 gives the nodes as zeros of $\varphi_n(x)$

weights as $w_j = \dfrac{-a_n \gamma_n}{\varphi_n'(x_j)\,\varphi_{n+1}(x_j)}$

where $\{\varphi_n(x) \mid n \geq 0\}$ are orthogonal polynomials on (a, b) with weight function $w(x) \geq 0$.

$$\gamma_n = \int_a^b w(x)\, \varphi_n(x)^2\, dx$$

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For interval $[a, b] = [-1, 1]$ & weight function $w(x) = 1$

$\Rightarrow$ $\varphi_n(x)$ is the Legendre polynomial

$P_0(x) = 1$

$P_n(x) = \dfrac{1}{n!\,2^n} \dfrac{d^n}{dx^n}\left[(x^2-1)^n\right]$ $n = 1, 2, \ldots$

Gaussian numerical integration gives the error

$$| I(f) - I_n(f) | \leq 2(b-a)\rho_{2n-1}(f)$$

where $\rho_{2n-1}(f)$ is the minimax error of degree $2n-1$ for $f(x)$ on $[a, b]$.

Weighted Gaussian Quadrature:

$$I(f) = \int_a^b w(x) f(x)\, dx \quad , \quad [a, b] = [0, 1]$$

say $w(x) = \frac{1}{\sqrt{x}}$

$$I(f) = \int_0^1 \frac{f(x)}{\sqrt{x}}\, dx$$

what if $w(x) = \frac{1}{\sqrt{1-x^2}}$?
what are the integration nodes?

Case $n=1$

$$\int_0^1 \frac{f(x)}{\sqrt{x}}\, dx \sim w_1 f(x_1)$$

$$f(x) = 1 \qquad \int_0^1 \frac{1}{\sqrt{x}}\, dx = w_1 \qquad w_1 = 2$$

$$f(x) = x \qquad \int_0^1 \frac{x}{\sqrt{x}}\, dx = w_1 x_1 \ , \quad x_1 = \frac{1}{3}$$

$$\boxed{\therefore \int_0^1 \frac{f(x)}{\sqrt{x}}\, dx \sim 2 f(\tfrac{1}{3})}$$

$x_{j,n} = \cos\left(\frac{2j-1}{2n}\pi\right)$

$w_{j,n} = \frac{\pi}{n}$

$$\int_{-1}^1 \frac{f(x)}{\sqrt{1-x^2}}\, dx = \frac{\pi}{n}\sum_{j=1}^{n} f(x_{j,n}) + \frac{2\pi}{2^{2n}(2n)!} f^{(2n)}(\eta)$$

Case $n=2$

$$\int_0^1 \frac{f(x)}{\sqrt{x}}\, dx \sim w_1 f(x_1) + w_2 f(x_2)$$

$f(x)=1$ $\quad \omega_1+\omega_2 = \int_0^1 \frac{1}{\sqrt{x}}\,dx = 2$

$f(x)=x$ $\quad \omega_1 x_1+\omega_2 x_2 = \int_0^1 \frac{x}{\sqrt{x}}\,dx = \frac{2}{3}$

$f(x)=x^2$ $\quad \omega_1 x_1^2+\omega_2 x_2^2 = \int_0^1 \frac{x^2}{\sqrt{x}}\,dx = \frac{2}{5}$

$f(x)=x^3$ $\quad \omega_1 x_1^3+\omega_2 x_2^3 = \int_0^1 \frac{x^3}{\sqrt{x}}\,dx = \frac{2}{7}$

$$x_1 = \frac{3}{7} - \frac{2}{35}\sqrt{30}$$

$$x_2 = \frac{3}{7} + \frac{2}{35}\sqrt{30}$$

$$\omega_1 = 1 + \frac{1}{18}\sqrt{30}$$

$$\omega_2 = 1 - \frac{1}{18}\sqrt{30}$$

Case $n>2$ $\Rightarrow$ formula be exact for the $2n$ monomials

$f(x) = 1,\ x,\ x^2,\ \dots,\ x^{2n-1}$

$2n$ unknowns

$2n$ equations (nonlinear)

~~Example~~:

$\boxed{\text{HW}}$: Consider the integral $I(f) = \int_0^1 f(x)\log\left(\frac{1}{x}\right)dx$

with $f(x)$ a function with several continuous derivatives on $0 \le x \le 1$.

(a) Find a formula

$$\int_0^1 f(x)\log\left(\frac{1}{x}\right)dx \approx w_1 f(x_1) \equiv I_1(f)$$

exact if $f(x)$ is any linear polynomial.

(b) Find a formula

$$\int_0^1 f(x)\log\left(\frac{1}{x}\right) \approx w_1 f(x_1) + w_2 f(x_2) \equiv I_2(f)$$

exact for all polynomials of degree ≤ 3.

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$$I - I_n = \frac{C_1}{n^{3/2}} + \frac{C_2}{n^2} + \frac{C_3}{n^{5/2}} + \frac{C_4}{n^3} + \cdots$$

$$I - I_{2n} = \frac{C_1}{(2n)^{3/2}} + \frac{C_2}{(2n)^2} + \frac{C_3}{(2n)^{5/2}} + \frac{C_4}{(2n)^3} + \cdots$$

$$I - I_{4n} = \frac{C_1}{(4n)^{3/2}} + \frac{C_2}{(4n)^2} + \frac{C_3}{(4n)^{5/2}} + \frac{C_4}{(2n)^3} + \cdots$$

three unknowns, three equations, and then substitute them into $I - I_n$ to ~~get~~ find a combination for an estimate of I with an error of order $1/n^{5/2}$

$$I_{2n} - I_n = \frac{1}{n^{3/2}}\left(1 - \frac{1}{2^{3/2}}\right)C_1 + \frac{1}{n^2}\left(1 - \frac{1}{2^2}\right)C_2$$

$$I_{4n} - I_n = \frac{1}{n^{3/2}}\left(1 - \frac{1}{2^2}\right)C_1 + \frac{1}{n^2}\left(1 - \frac{1}{4^2}\right)C_2$$

find C_1 & C_2 in terms of I_n, I_{2n} & I_{4n}

Numerical Differentiation

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

numerically, $f'(x) \sim \dfrac{f(x+h) - f(x)}{h} = D_h f(x)$ forward difference

or

$f'(x) \sim \dfrac{f(x) - f(x-h)}{h}$ backward difference

$$f(x+h) \sim f(x) + h f'(x)$$

$f(x+h) = f(x) + h f'(x) + \frac{h^2}{2} f''(c)$ for some c between x & $x+h$

$$D_h f(x) = \frac{f(x) + h f'(x) + \frac{h^2}{2} f''(c) - f(x)}{h}$$

$$= f'(x) + \frac{h}{2} f''(c)$$

$f'(x) - D_h f(x) = -\frac{h}{2} f''(c)$ $\Rightarrow$ error is proportional to h

Differentiation using interpolation

$$f(x) \sim P_n(x) = \sum_{j=0}^{n} f(x_j)\, l_j(x)$$

$$l_j(x) = \frac{\Psi_n(x)}{(x-x_j)\,\Psi_n'(x_j)}$$

$$\Psi_n(x) = (x-x_0)(x-x_1)\cdots(x-x_n)$$

$$f(x) - P_n(x) = \Psi_n(x)\, f[x_0, x_1, \cdots, x_n, x]$$

$$f'(x) \sim P_n'(x) \equiv D_n f(x)$$

$$f'(x) - D_n f(x) = \Psi_n'(x) f[x_0, x_1, \cdots, x_n, x]$$

$$+ \Psi_n(x) f[x_0, x_1, \cdots x_n, x, x]$$

$$= \Psi_n'(x) \frac{f^{(n+1)}(\xi_1)}{(n+1)!} + \Psi_n(x) \cdot \frac{f^{(n+2)}(\xi_2)}{(n+2)!}$$

assume evenly spaced nodes :

$$x_i = x_0 + ih,$$

recall that $|\Psi_n(x)| \leq n!\, h^{n+1}$ for $a \leq x \leq b$

$|\Psi_n'(x)| \leq n \cdot (n-1)!\, h^n$ for $a \leq x \leq b$

$$\therefore \quad f'(x) - D_n f(x) = \begin{cases} O(h^n) & \Psi_n'(x) \neq 0 \\ O(h^{n+1}) & \Psi_n'(x) = 0 \end{cases}$$

varying n & varying the placement of the nodes relative to the point t of interest, we can write down many different formulas for numerical diff.

For example: $n=1$

$$f'(x_0) \approx D_h f(x_0) \equiv \frac{1}{h}\left[f(x_0+h) - f(x_0) \right]$$

forward difference formula

$n=2$, $\quad x = x_1$, $\quad x_0 = x_1 - h$, $\; x_2 = x_1 + h$

$$P_2'(x_1) = \frac{f(x_2) - f(x_0)}{2h} = \frac{f(x_1+h) - f(x_1-h)}{2h} \equiv D_h f(x_1)$$

$\Rightarrow$ central difference formula

Method of undetermined coefficients

write $f''(t) \approx D_h^{(2)} f(t) \equiv A f(t+h) + B f(t) + C f(t-h)$

$$f(t-h) \approx f(t) - h f'(t) + \frac{h^2}{2} f''(t) - \frac{h^3}{6} f^{(3)}(t) + \frac{h^4}{4!} f^{(4)}(t)$$

$$f(t+h) \approx f(t) + h f'(t) + \frac{h^2}{2} f''(t) + \frac{h^3}{6} f^{(3)}(t) + \frac{h^4}{4!} f^{(4)}(t)$$

$$D_h^{(2)} f(t) = A\, f(t+h) + B\, f(t) + C f(t-h)$$

$$= A\cdot\left(f(t) + h f'(t) + \frac{h^2}{2} f''(t) + \frac{h^3}{6} f^{(3)}(t) + \frac{h^4}{4!} f^{(4)}(t)\right)$$

$$+ B\ f(t)$$

$$+ C\left(f(t) - h f'(t) + \frac{h^2}{2} f''(t) - \frac{h^3}{6} f^{(3)}(t) + \frac{h^4}{4!} f^{(4)}(t)\right)$$

$$= (A+B+C)\, f(t)$$

$$+ h(A-C)\ f'(t)$$

$$+ \frac{h^2}{2}(A+C)\ f''(t)$$

$$+ \frac{h^3}{3!}(A-C)\ f^{(3)}(t)$$

$$+ \frac{h^4}{4!}(A+C)\ f^{(4)}(t)$$

$$\Rightarrow \quad A+B+C=0 \qquad \Rightarrow \quad A = C = \frac{1}{h^2} \qquad B = -\frac{2}{h^2}$$

$$A - C = 0$$

$$\frac{h^2}{2}(A+C) = 1$$

$$\therefore \quad D_h^{(2)} f = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

the error estimate: $D_h^{(2)} f = f''(x) + \frac{h^2}{12} f^{(4)}(x)$