Numerical Integration (Quadrature)

Definite Integral of $f(x)$

$$\boxed{I_f = \int_a^b f(x)dx \approx \sum_{i=0}^{n} a_i f(x_i)}$$

a_i are called the quadrature weights

Some integrals are difficult or impossible to do analytically

Assume that function values $f(x_i)$ are known on a set of discrete points $x_0 = a, x_1, x_2, \dots x_n = b$

Several rules or methods for numerical integration are available

We will aim for high accuracy

Basic Quadrature Rules

Based on low degree polynomial interpolation

$$\boxed{I_f = \int_a^b f(x)dx \approx \int_a^b p_n(x)dx}$$

Let us consider the Lagrange polynomial for $p_n(x)$

$$p_n(x) = \sum_{i=0}^{n} f(x_i)L_i(x)$$

$$L_i(x) = \prod_{\substack{k=0 \\ i\neq k}}^{n} \frac{(x - x_k)}{(x_i - x_k)} = \frac{(x - x_0)\ldots(x - x_{i-1})(x - x_{i+1})\ldots(x - x_n)}{(x_i - x_0)\ldots(x_i - x_{i-1})(x_i - x_{i+1})\ldots(x_i - x_n)}$$

$$\boxed{I_f = \int_a^b f(x)dx \approx \int_a^b p_n(x)dx = \int_a^b \sum_{i=0}^{n} f(x_i)L_i(x)}$$

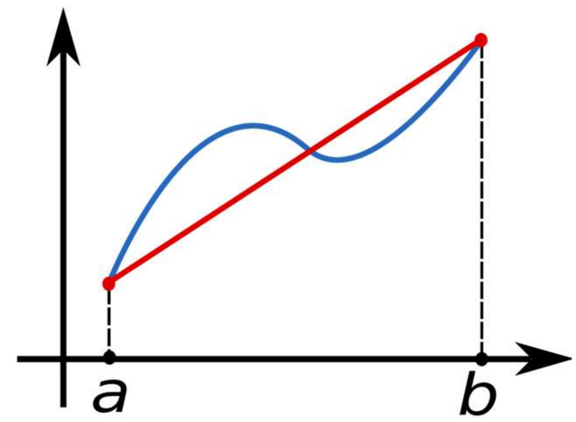
$$I_f \approx \sum_{i=0}^{n} f(x_i) \int_a^b L_i(x)dx$$

Quadrature weights: $a_i = \int_a^b L_i(x)dx$

Quadrature weights are precomputed *once and for all* as part of constructing a *quadrature rule*

Trapezoidal Rule

Set *n=1* and interpolate at $x_0 = a \quad \& \quad x_1 = b$



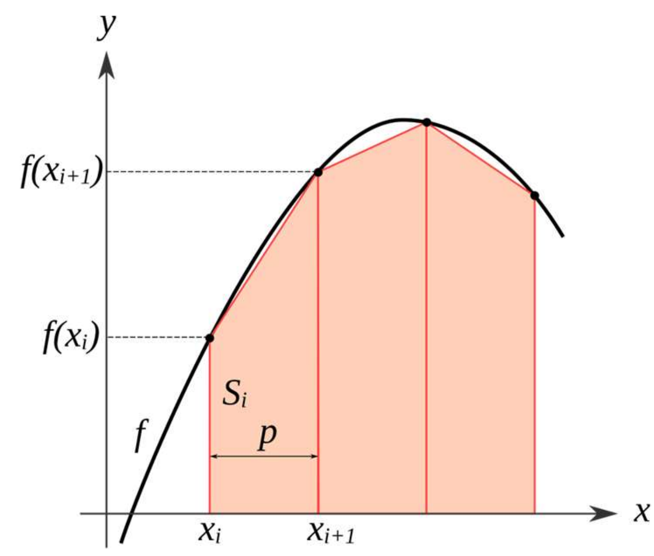
$$L_0 = \frac{x-a}{a-b}, \qquad L_1 = \frac{x-a}{b-a}$$

The quadrature weights are

$$a_0 = \int_a^b L_0(x)dx = \frac{b-a}{2}, \qquad a_1 = \int_a^b L_1(x)dx = \frac{b-a}{2}$$

$$I_f \approx I_{trap} = \sum_{i=0}^{n} f(x_i) \int_a^b L_i(x)dx = a_0 f(a) + a_1 f(b)$$

$$\boxed{I_{trap} = \frac{b-a}{2}[f(a) + f(b)]}$$



Simpson's Rule (1/3 rule)

Set *n=2* and interpolate at $x_0 = a, \quad x_1 = \frac{a+b}{2}, \quad x_2 = b$

$$\boxed{I_{Simp} = \frac{b-a}{6}\left[f(a) + 4f\left(\frac{b+a}{2}\right) + f(b)\right]}$$

Note that abscissae x_0, x_1, x_2 are chosen to be equidistant.

Simpson's 3/8 rule uses four points with n=3, but it is not much accurate than 1/3 rule. Therefore, 1/3 rule is often the preferred method.

Composite Simpson's 1/3 Rule

When an interval [a,b] is subdivided into n intervals, we can apply the integration rule to each interval and add up the results, which is known as *composite* or *compound* integral.

For a single interval:

$$I_{Simp} = \frac{b-a}{6}\left[f(a) + 4f\left(\frac{b+a}{2}\right) + f(b)\right]$$

Composite rule for the entire interval

$$I_{Simp} = \frac{h}{3}\left[f(x_0) + 4\sum_{\substack{i=1 \\ i=odd}}^{n-1} f(x_i) + 2\sum_{\substack{i=2 \\ i=even}}^{n-2} f(x_i) + f(x_n)\right]$$

$$\boxed{h = x_{i+1} - x_i, \qquad x_0 = a, \qquad x_n = b}$$

Gauss Quadrature

Can we choose abscissae x_0, x_1, x_2 judiciously to improve accuracy?

$$I_f = \int_a^b f(x)dx \approx \sum_{i=0}^{n} a_i f(x_i)$$

Now instead of integrating the interpolant, let us try to maximize the degree of the polynomial f that we can integrate the interpolant exactly.

Choose *n+1* points $\{x_i\}_{i=0}^{n}$. Can we increase the precision to *2n+1?*

Choose the abscissae as the roots (zeros) of the Legendre polynomials → Gauss points

Once the Gauss points are determined, compute quadrature weights by integrating the Lagrange polynomials

Legendre Polynomials

$x \in [-1,1]$

$$\phi_0(x) = 1, \qquad \phi_1(x) = x$$

$$\phi_{j+1}(x) = \frac{2j+1}{j+1} x\phi_j(x) - \frac{j}{j+1}\phi_{j-1}(x), \qquad j \geq 1.$$

$$\phi_0(x) = 1,$$

$$\phi_1(x) = x,$$

$$\phi_2(x) = \frac{1}{2}(3x^2 - 1),$$

$$\phi_3(x) = \frac{1}{2}(5x^3 - 3x), \ldots$$

Gauss-Legendre Quadrature (Gauss Integration)

General quadrature rule $$I_f \approx \sum_{i=0}^{n} f(x_i) \int_a^b L_i(x)dx$$

Quadrature weights: $$a_i = \int_a^b L_i(x)dx$$

Consider a polynomial of degree n=1 to interpolate f(x) at n+1=2 points

Abscissae are the roots of the n+1=2 Legendre polynomial $\phi_2(x) = \frac{1}{2}(3x^2 - 1)$,

$$x_0 = -\sqrt{\frac{1}{3}}, \qquad x_1 = \sqrt{\frac{1}{3}}$$

Quadrature weights: $a_o = \int_{-1}^{+1} L_0(x)dx = 1, \qquad a_1 = \int_{-1}^{+1} L_1(x)dx = 1$

$$\int_{-1}^{+1} f(x)dx \approx \sum_{i=0}^{n} a_i f(x_i) = f\left(-\sqrt{1/3}\right) + f\left(\sqrt{1/3}\right)$$

Gauss-Legendre Quadrature

On the interval [-1, 1]

Gauss points are the roots (zeros) of the Legendre polynomial of degree n+1 $\phi_{n+1}(x)$

Quadrature weights $a_j = \frac{2(1-x_j^2)}{\left[(n+1)\phi_n(x_j)\right]^2}, \quad j = 0,1,\ldots n.$

For a general interval $t \in [a, b]$, we use the following affine transformation

$$t = \frac{b-a}{2}x + \frac{b+a}{2}, \qquad -1 \le x \le 1$$

$$dt = \frac{b-a}{2}dx$$

Gauss-Lobatto (Radau) Quadrature

Evaluate integral of the following form when choice of abscissae is not entirely free e.g. some points can be fixed.

$$\int_{-1}^{+1} f(x)dx$$

Useful in the solution of stiff differential equations

Gauss-Hermite Quadrature

Evaluate integral of the following form

$$\int_{-\infty}^{+\infty} e^{-x^2} f(x)dx$$

Leads to accurate results provided that $f(x)$ grows slower than e^{x^2} as |x| approaches ∞

General approach (not always numerically stable)

$$\int_{-\infty}^{+\infty} f(x)dx = \int_{-\infty}^{+\infty} e^{-x^2} e^{x^2} f(x)dx = \int_{-\infty}^{+\infty} e^{-x^2} g(x)dx$$

Gauss-Laguerre Quadrature

Evaluate integral of the following form

$$\int_0^{+\infty} e^{-x} f(x)dx$$

Leads to accurate results provided that $f(x)$ grows slower than e^{x^2} as |x| approaches ∞

Chebyshev-Gauss Quadrature

Evaluate integral of the following form

$$\int_0^{+\infty} e^{-x} f(x)dx$$

Leads to accurate results provided that $f(x)$ grows slower than e^{x^2} as |x| approaches ∞

Error in Composite Gaussian Quadrature

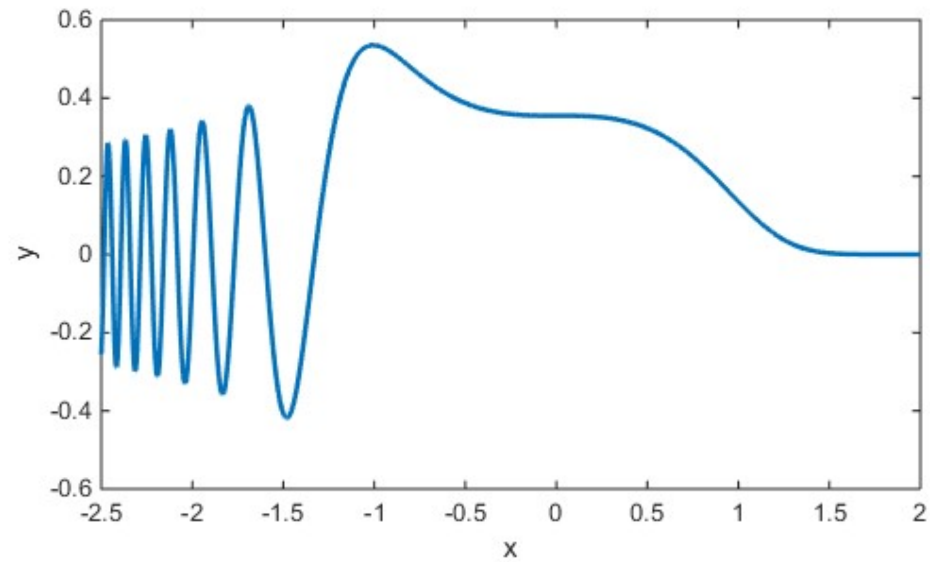
$$\boxed{I_f = \int_a^b f(x)dx \approx \sum_{i=0}^{n} a_i f(x_i)}$$

For n+1 Gauss points

$$e_{n,h}(f) = \frac{(b-a)\big((n+1)!\big)^4}{(2n+3)\big((2n+2)!\big)^2} f^{(2n+2)}(\xi) h^{2n+2}$$

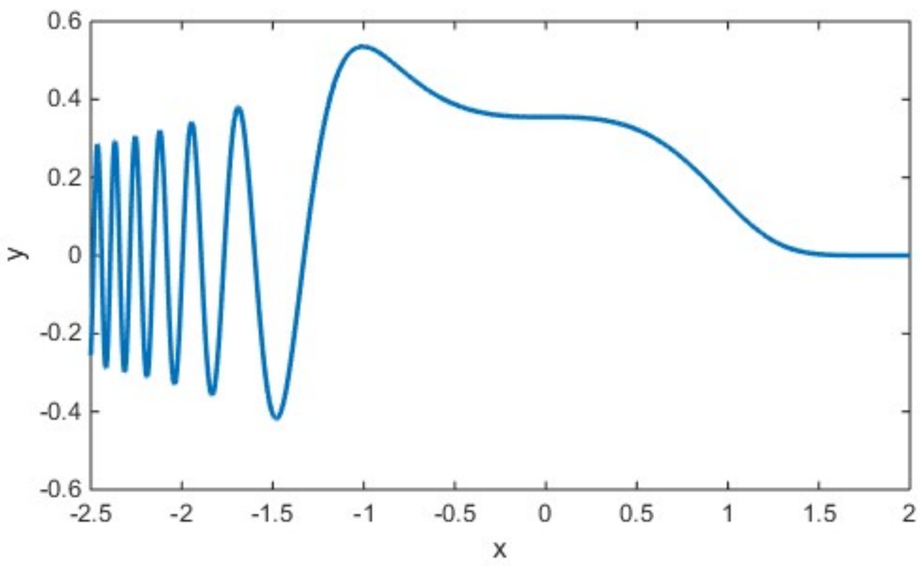
Adaptive Quadrature

- Some functions vary faster in one part of the domain compared to another
- An extreme example is shown at right
- We would want to put more nodes to interpolate accurately where there is rapid oscillation (imagine using PL interp)
- It is similar for integration: more points needed where there is fast variation



Adaptive Quadrature

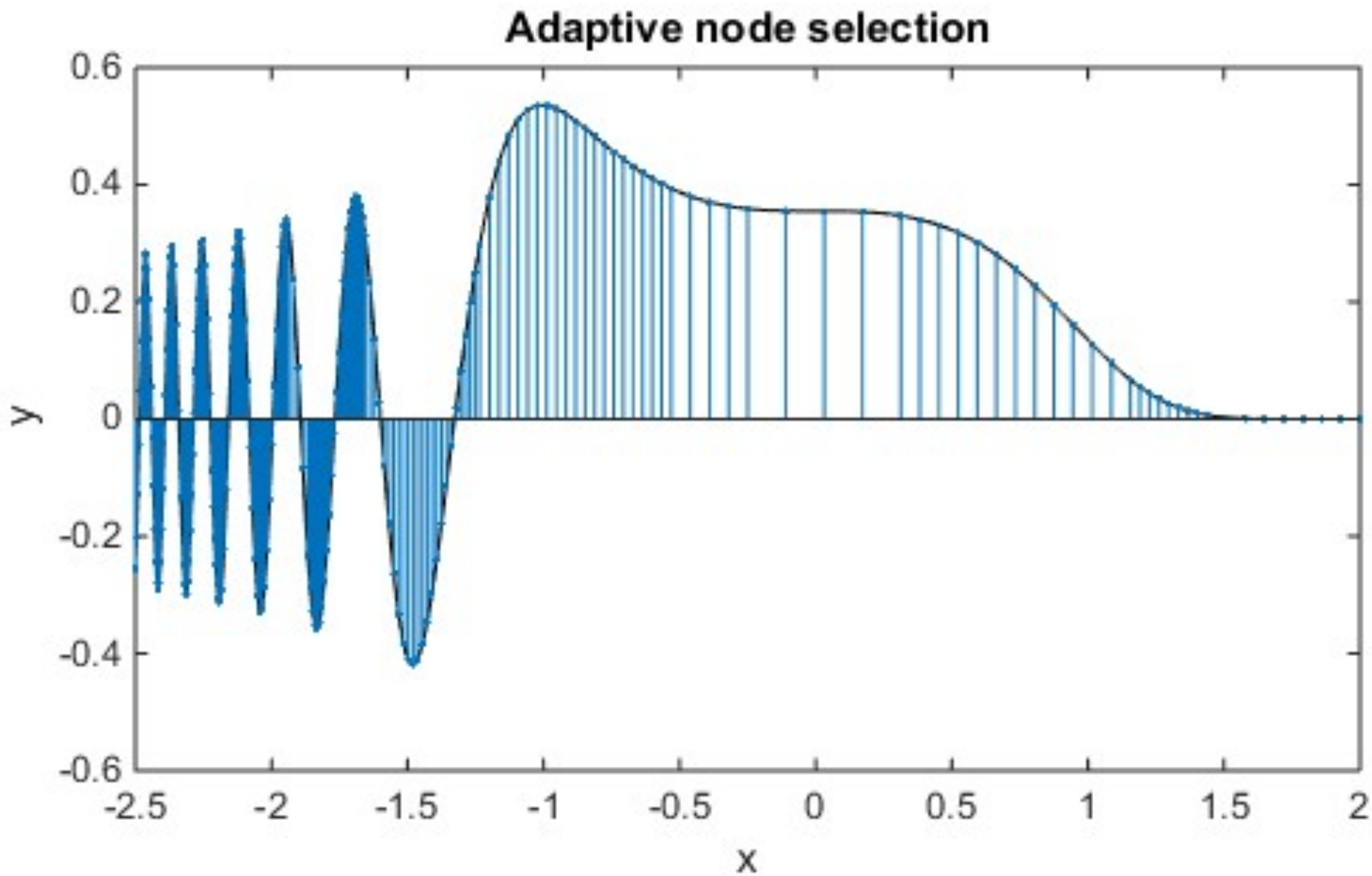
- Strategy: estimate error using knowledge of Simpson rule
- Start by one and two intervals over whole domain
- Apply Simpson rule on all intervals
- Estimate error; if larger than tolerance, then subdivide again in half that did not satisfy tolerance (could be one or both)
- Recursively do this in each subdomain



Adaptive Quadrature

- Simpson rule error is $O(h^4)$
- For one interval, $I = S_1 + Ch^4$
- For two intervals over same limits, $I = S_2 + Ch^4/16$
- We assume C is same for both, but we don't know it
- Subtract the two, and solve for Ch^4
- This gives estimate for error: $\mathrm{E} \approx Ch^4 = \frac{S_1 - S_2}{15} = \delta$
- We compute S_1 and S_2, from the method, then use them to estimate the error
- If $\delta > tol$, then subdivide the interval by calling `your function` again (apply the test again with subdivision)

Adaptive Quadrature Example



Multiple Integrals

$$I = \iint\limits_{A} f(x,y)dA = \int_{a}^{b}\left[\int_{y=g(x)}^{y=p(x)} f(x,y)dy\right]dx$$

Same rules that we have covered applies.
Apply the rules to the inner integral over dx,
then apply the rules to the outer integral over dy

Improper Integrals

Improper Integral: interval of integration or integrand itself is unbounded

$$\int_{-\infty}^{+\infty} f(x)dx \approx \int_{-M}^{+M} f(x)dx \approx$$

Strategies:

1. Use a standard quadrature rule on a finite interval. Choose *M* wisely such that omitted tails of the function are negligible
2. Use a quadrature rule designed for an unbounded interval (e.g. Gauss-Laguerre, Gauss-Hermite)
3. Transform the variable of integration so that the new interval is finite

$$x = -\log t \quad or \quad x = \frac{t}{t-1}$$

Integrands with Singularities

Example: $\int_0^{\frac{\pi}{2}} \frac{\cos(x)}{\sqrt{x}} dx$

Under the transformation $x = t^2$

$$\int_0^{\sqrt{\frac{\pi}{2}}} \frac{\cos(t^2)}{t} (2t) dt = \int_0^{\sqrt{\frac{\pi}{2}}} \cos t^2 \, dt$$

There is no established rule to eliminate singularities. A bit of an art!

Integral Equations

Unknown to be determined is a *function* inside the integral sign

$$\int_a^b K(s,t)u(t)dt = f(s)$$

where K is the kernel, f is a known function, and u to be found.

Can be viewed as a continuous analogue of a system of algebraic equations $\mathbf{A}x = y$

Very common in science & engineering

K represents the response function of an instrument, f represents measured data, u is the underlying signal to be determined.

Approximation to the integral equation: $$\sum_{j=1}^{n} w_j K(s_i, t_j) u(t_j) = f(s_i)$$

$i=1,2,\ldots,n$

Integral Equations

Approximation leads to a system of linear algebraic equations $\mathbf{A}x = y$, which is often ill-conditioned

Example: $\int_{-1}^{+1}(1 + \alpha st)u(t)dt = 1$

Use composite midpoint rule with two subintervals $t_1 = -\frac{1}{2},\ t_2 = \frac{1}{2}$ and $w_1 = w_2 = 1$

Choose $s_1 = -\frac{1}{2},\ \ s_2 = \frac{1}{2}$

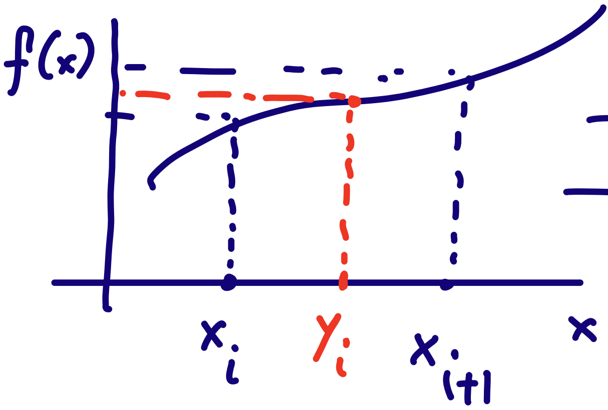
$$Ax = \begin{bmatrix} 1 + \dfrac{\alpha}{4} & 1 - \dfrac{\alpha}{4} \\ 1 - \dfrac{\alpha}{4} & 1 + \dfrac{\alpha}{4} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$x = \begin{bmatrix} \dfrac{1}{2} & \dfrac{1}{2} \end{bmatrix}^T$$

Solution is independent of α. The ill-conditioning of matrix A can be shown by varying α

More accurate quadrature rules makes the conditioning worse!

Error Analysis.



mid-point (rectangle) rule

$$I = \int_{x_i}^{x_{i+1}} f(x)\,dx \approx h_i\, f(y_i)$$

$h_i = x_{i+1} - x_i$

$y_i = \dfrac{x_i + x_{i+1}}{2}$ mid point

Taylor Series of $f(x)$ about y_i

$$f(x) = f(y_i) + (x - y_i)\, f'(y_i) + \frac{1}{2}(x - y_i)^2 f''(y_i) + \frac{1}{6}(x - y_i)^3 f'''(y_i) + \cdots$$

$$f(y_i) = f(x_i) - (x_i - y_i)\, f'(y_i) - \cdots$$

$$I = \int_{x_i}^{x_{i+1}} f(x)\,dx \approx x\, f(y_i)\Big|_{x_i}^{x_{i+1}} + \frac{(x - y_i)^2}{2}\, f'(y_i)\Big|_{x_i}^{x_{i+1}} + \frac{1}{6}(x - y_i)^3\Big|_{x_i}^{x_{i+1}} \overset{2}{f''}(y_i) + $$

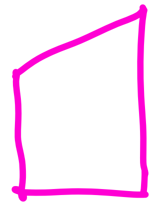
even powers of $(x - y_i)^n$ vanish. $\rightarrow 0$

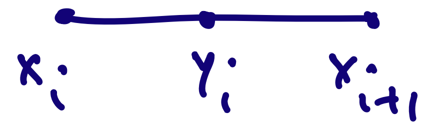
$h_i = (x_{i+1} - x_i)$

$$\int_{x_i}^{x_{i+1}} f(x)\,dx \approx h_i f(y_i) + \frac{h^3}{24} f''(y_i) + \frac{1}{1920} h^5 f^{IV}(y_i) + \cdots$$

mid-point rule is 3rd order accurate for one interval!

Trapezoid Rule





$$f(x_i) = f(y_i) - \frac{1}{2} h f'(y_i) + \frac{1}{8} h^2 f''(y_i) - \frac{1}{48} h^3 f'''(y_i) + \cdots$$

$$f(x_{i+1}) = f(y_i) + \frac{1}{2} h f'(y_i) + \frac{1}{8} h^2 f''(y_i) + \frac{1}{48} h^3 f'''(y_i) + \cdots$$

Trapezoid Rule $\quad \dfrac{f(x_{i+1}) + f(x_i)}{2}$

$$= f(y_i) + \frac{1}{8} h^2 f''(y_i) + \frac{1}{384} h^4 f(y_i)$$

from midpoint

$$\int_{x_i}^{x_{i+1}} f(x)\,dx \approx h f(y_i) + \frac{h^3}{24} f''(y_i) + \frac{1}{1920} h^5 f^{iv}(y_i) + \cdots$$

$$I \approx h_i \underbrace{\left(\frac{f(x_i) + f(x_{i+1})}{2} \right)}_{f(y_i)} - \frac{1}{12} h^3 f''(y_i) - \frac{1}{480} h^5 f^{IV}(y_i)$$

Trapezoid Rule for one interval is 3^{rd} order

For the entire interval $[a, b]$

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} f(x)\,dx$$

$$I_{ab} = \frac{h}{2}\left(f(a) + f(b) + 2\sum_{i=1}^{n-1} f_i \right)$$

$$- \frac{h^3}{12}\sum_{i=0}^{n-1} f''(y_i) + \cdots$$

Mean Value Theorem

$$\int_a^b f(x)\,dx = f(\bar{x})(b-a)$$

$$\sum f(x_i)\,h \simeq \int_a^b f(x)\,dx$$

$$\sum f(x_i) = \frac{f(\bar{x})(b-a)}{h}$$

order of accuracy comes down to

2^{nd} (

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Richardson Extrapolation.

* builds on the knowledge of truncation error.

$$I = \int_a^b f(x)\,dx \quad \text{(exact)}$$

approximation $\tilde{I}$

$$I = \tilde{I} + c_1 h^2 + c_2 h^4 + c_3 h^6 \ldots$$

$$\tilde{I}_1 = I - c_1 h^2 - c_2 h^4 - c_3 h^6 - \ldots$$

now halve the interval size

$h \longrightarrow h/2$

$$\tilde{I}_2 = I - c_1 \frac{h^2}{4} - c_2 \frac{h^4}{16} - c_3 \frac{h^6}{64}$$

to eliminate $O(h^2)$ terms.

$$\tilde{I}_{12} = \frac{4\tilde{I}_2 - \tilde{I}_1}{3} = I + \frac{1}{4} c_2 h^4 + \frac{5}{16} c_3 h^6$$

$\tilde{I}_{12}$ 4^{th} order accurate.

let's use $\frac{h}{2}$ & $\frac{h}{4}$

$\tilde{I}_2$, $\tilde{I}_3$ both are 2^{nd} order

$$\tilde{I}_{23} = \frac{4\tilde{I}_3 - \tilde{I}_2}{3}$$

come up with a linear combination of $\tilde{I}_{23}$ & $\tilde{I}_{12}$

$\rightarrow$ 6^{th} order method

$\rightarrow$ can go on indefinitely

$\rightarrow$ Romberg Integration.

Error in polynomial interpolation.

$f(x)$ defined in $[a, b]$

$$e_n = f(x) - P_n(x)$$

for any point in $[a, b]$

assume derivatives of $f(x)$ exist & bounded in $[a, b]$

$[x_i, y_i]$ $i = 0, 1, 2 \ldots n$

$(n+1)$ points

a useful method is Newton's polynomial.

$$p_{n+1}(x) = p_n(x) + f[x_0, x_1 \dots x_n, x_{n+1}] * \prod_{i=0}^{n} (x - x_i)$$

$$p_n(x) = p_{n+1}(x) - f[\dots] \prod_{i=0}^{n} (x - x_i)$$

$$e_n(x) = \underbrace{f[x_0 \dots x_n, x]}_{\text{divided difference}} \prod_{i=0}^{n} (x - x_i)$$

$f(x)$ has $n+1$ bounded derivative

$\xi \in [a, b]$

$$e_n(x) = f(x) - p_n(x) = \frac{f^{n+1}(\xi)}{(n+1)!} \prod_{i=0}^{n} (x - x_i)$$

divided difference

$$f[x_i, \ldots x_j] = \frac{f^{n+1}(\xi)}{(n+1)!}$$

$$= \frac{f[x_{i+1} \ldots x_j] - f[x_i \ldots x_{j-1}]}{x_j - x_i}$$

which is recursive

example:

$$\underbrace{f[x_0, x_1]}_{\text{divided difference for } f'} = \frac{f(x_1) - f(x_0)}{x_1 - x_0} = f'(x_0)$$