Nonlinear Equations

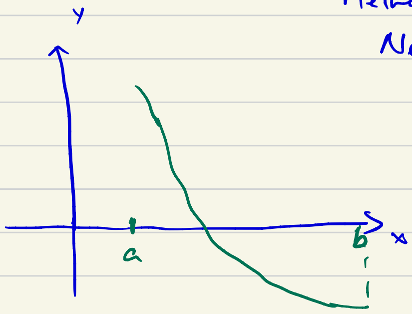
$f(x) = 0$ $\qquad x \in [a, b]$

Method of false posn ← Regula falsi

Newtons method ← Newton-Raphson

Bisection

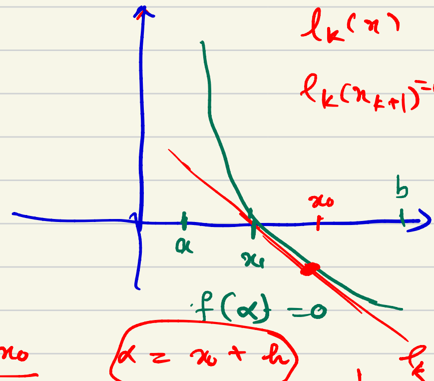
Secant



$f(a)\,f(b) < 0 \qquad c = \dfrac{a+b}{2}$

$f(a)\,f(c) < 0$

$f(b)\,f(c) < 0$



$f(\alpha) = 0$

$h = \alpha - x_0 \qquad \alpha = x_0 + h$

$0 = f(x_0 + h) = f(x_0) + h f'(x_0) + R_n(x_0, \xi)$

$0 = f(x_0 + h) \approx f(x_0) + h f'(x_0)$

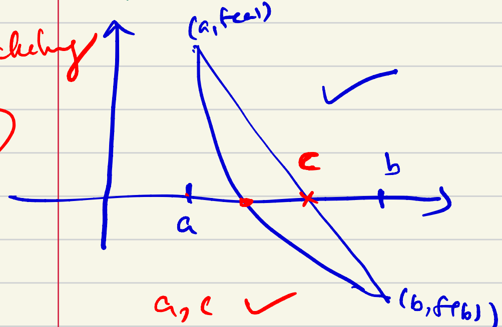
$x_1 = x_0 + h \approx \alpha$

$h = \dfrac{-f(x_0)}{f'(x_0)}$

$x_1 = x_0 - \dfrac{f(x_0)}{f'(x_0)}$

Regula Falsi method

Bracketing



a, c

c, b

Formula same.

Secant Method

No bracket $\quad x_{k+1} = x_k - \dfrac{f(x_k)}{f'(x_k)}$

$f'(x_k) \approx \dfrac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}}$

$= x_k - \dfrac{f(x_k)}{}$

$$\begin{cases} e_{k+1} = \alpha - x_{k+1} = c(\alpha - x_k)^2 = c e_k^2 \quad \text{(Newtons)} \to \text{quadratic} \\ e_{k+1} = c_1 e_k^{1.63} \to \text{superlinear} \quad \text{(secant)} \end{cases}$$

Non-linear system

$$(1) \quad \begin{cases} f_1(x_1, x_2, \dots x_n) = 0 \\ f_2(x_1, x_2, \dots x_n) = 0 \\ \vdots \\ f_n(x_1, x_2 \dots x_n) = 0 \end{cases}$$

$\bar{F} = [f_1 \ f_2 \ \dots \ f_n]^T$

$\bar{x} = [x_1 \ x_2 \ \dots \ x_n]^T$

$\bar{F}(\bar{x}) = \bar{0}$

$x_1, x_2 \dots x_n$ are indep variables

$$f_i : \mathbb{R}^n \to \mathbb{R}$$

$$\bar{F} : \mathbb{R}^n \to \mathbb{R}^n$$

Newton's method Let $\bar{\alpha} = (\alpha_1, \alpha_2 \dots \alpha_n)$ be an exact soln of $\bar{F}(\bar{x}) = \bar{0}$

i.e. $\bar{F}(\bar{\alpha}) = \bar{0}$ If $\bar{x}^{(0)} \in \mathbb{R}^n$ be an inial guen. $\bar{\alpha} = \bar{x}^{(0)} + \bar{h}$

$$\bar{F}(\bar{x}^{(0)} + \bar{h}) = \bar{0}$$

$$f_i(\bar{\alpha}) = 0 \qquad i = 1, 2 \dots n$$

$$\Rightarrow f_i(\bar{x}^{(0)} + \bar{h}) = 0 \qquad (2)$$

$$\bar{h} = [h_1 \ h_2 \ \cdots \ h_n]^T$$

$$\bar{f}_i' = \left[\frac{\partial f_i}{\partial x_1} \ \cdots \ \frac{\partial f_i}{\partial x_n}\right]^T_{\bar{x}^{(0)}}$$

$$0 = f_i(\bar{\alpha}) = f_i(\bar{x}^{(0)} + \bar{h})$$

$$= f_i(\bar{x}^{(0)}) + \bar{h} \cdot \bar{f}_i'(\bar{x}^{(0)}) + R_n(\bar{x}^{(0)}, \bar{\xi}_i)$$

$$0 = f_i(\bar{x}^{(0)}) + \left(h_1 \left.\frac{\partial f_i}{\partial x_1}\right|_{\bar{x}^{(0)}} + \cdots + h_n \left.\frac{\partial f_i}{\partial x_n}\right|_{\bar{x}^{(0)}}\right) + \underbrace{O(h_1^2 \cdots h_n^2)}$$

$$0 \approx f_i(\bar{x}^{(0)}) + \left(h_1 \left.\frac{\partial f_i}{\partial x_1}\right|_{\bar{x}^{(0)}} + \cdots + h_n \left.\frac{\partial f_i}{\partial x_n}\right|_{\bar{x}^{(0)}}\right)$$

$i = 1, 2 \cdots n$

$$h_1^{(0)} \left.\frac{\partial f_i}{\partial x_1}\right|_{\bar{x}^{(0)}} + \cdots + h_n^{(0)} \left.\frac{\partial f_i}{\partial x_n}\right|_{\bar{x}^{(0)}} \approx -f_i(\bar{x}^{(0)})$$

$i = 1, 2 \cdots n$

$$\underbrace{\begin{bmatrix} \partial f_1/\partial x_1 & \cdots & \partial f_1/\partial x_n \\ \partial f_2/\partial x_1 & \cdots & \partial f_2/\partial x_n \\ - & - & - \\ \partial f_n/\partial x_1 & \cdots & \partial f_n/\partial x_n \end{bmatrix}_{\bar{x}^{(0)}}}_{J^{(0)} \ \text{Jacobian.}} \begin{bmatrix} h_1^{(0)} \\ h_2^{(0)} \\ \vdots \\ h_n^{(0)} \end{bmatrix} = \underbrace{\begin{bmatrix} -f_1(\bar{x}^{(0)}) \\ -f_2(\bar{x}^{(0)}) \\ \vdots \\ -f_n(\bar{x}^{(0)}) \end{bmatrix}}_{-F(\bar{x}^{(0)}) = -F^{(0)}} \quad (3)$$

solve (3) for $\bar{h}^{(0)} = [h_1^{(0)} \ h_2^{(0)} \ \cdots \ h_n^{(0)}]^T$

$$\bar{\alpha} \approx \bar{x}^{(1)} = \bar{x}^{(0)} + \bar{h}^{(0)} = \bar{x}^{(0)} - J^{(0)^{-1}} \bar{F}^{(0)}$$

$$\begin{cases} \bar{x}^{(k+1)} = \bar{x}^{(k)} + \bar{h}^{(k)} \\ \text{where} \quad J^{(k)} \bar{h}^{(k)} = -\bar{F}^{(k)} \\ J^{(k)} = \left(\partial f_i / \partial x_j \Big|_{\bar{x}^{(k)}} \right) \end{cases}$$

$A = (a_{ij})$

$$\bar{F}^{(k)} = \begin{bmatrix} f_1(\bar{x}^{(k)}) \\ \vdots \\ f_n(\bar{x}^{(k)}) \end{bmatrix}$$

Eg:

$$f_1(x,y) = xy + x^2 - y^3 - 1 = 0$$

$$f_2(x,y) = x + 2y - xy^2 - 2 = 0$$

$$(x^{(0)}, y^{(0)}) = (1/2, 1/2)$$

$$\bar{J}^{(k)} = \begin{bmatrix} \partial f_1/\partial x & \partial f_1/\partial y \\ \partial f_2/\partial x & \partial f_2/\partial y \end{bmatrix} = \begin{bmatrix} y + 2x & x - 3y^2 \\ 1 - y^2 & 2 - 2xy \end{bmatrix}$$

2^2

$$J^{(0)} = \begin{bmatrix} 3/2 & -1/4 \\ 3/4 & 3/2 \end{bmatrix}$$

$$J^{(0)^{-1}} = \frac{1}{2.4375} \begin{bmatrix} 1.5 & 0.25 \\ -0.75 & 1.5 \end{bmatrix} = \frac{16}{39} \begin{bmatrix} 3/2 & 1/4 \\ -3/4 & 3/2 \end{bmatrix}$$

$$\bar{h}^{(0)} = J^{(0)^{-1}} \left(-F^{(0)} \right)$$

$$\bar{F}^{(0)} = \begin{bmatrix} f_1(\bar{x}^{(0)}) \\ f_2(\bar{x}^{(0)}) \end{bmatrix} = \begin{bmatrix} -0.625 \\ -0.625 \end{bmatrix}$$

$$\bar{h}^{(0)} = \frac{-1}{2.4375}\begin{bmatrix} 1.5 & 0.25 \\ -0.75 & 1.5 \end{bmatrix}\begin{bmatrix} -0.625 \\ -0.625 \end{bmatrix}$$

$$= \begin{bmatrix} 0.4487 \\ 0.1923 \end{bmatrix}$$

$$\bar{x}^{(1)} = \bar{x}^{(0)} + \bar{h}^{(0)} = \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix} + \begin{bmatrix} 0.4487 \\ 0.1923 \end{bmatrix}$$

$$= \begin{bmatrix} 0.9487 \\ 0.6923 \end{bmatrix}$$

HW Find $J^{(1)}$, $\bar{F}^{(1)}$ and $\bar{h}^{(1)}$ so that

$$\bar{x}^{(2)} = \bar{x}^{(1)} + \bar{h}^{(1)} = \begin{bmatrix} 0.9019 \\ 0.9046 \end{bmatrix}$$

Exact $\alpha = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$

(quadratic convergence)

$$\bar{x}^{(k+1)} = \bar{x}^{(k)} - J_k^{-1} \bar{F}^{(k)}$$

Limitations of Newton's method

(1) At every iteration, Jacobian matrix $(J^{(k)})$ and and function values $(\bar{F}^{(k)})$ need to be calculated (n^2+n)

(2) Evaluation of analytical derivatives may not be feasible or slower the computation.

(3) Solving a linear system at every iteration. ($O(n^3)$ operations for GE)

Secant method $\quad f(x) = 0 \qquad f'(x) \approx \dfrac{f(x+h) - f(x)}{h}$

$$f'(x_k) \approx \frac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}}$$

Note

$$\frac{\partial f_i}{\partial x_j}(\bar{x}^{(k)}) \approx \frac{f_i(x_1, x_2 \cdots, x_j + h, \cdots x_n) - f_i(x_1, \cdots x_n)}{h}$$

$$\boxed{\begin{array}{l} \bar{x} = (x_1, x_2 \cdots x_n) \\ f_i(x_1, x_2 \cdots x_n) \end{array}}$$

n^2 such derivative calculations.

$$= \frac{f_i(\bar{x} + h\bar{e}_j) - f_i(\bar{x})}{h}$$

$i, j = 1, 2 \cdots n$

Broyden's method (A quasi-Newton method)

* Generalization of secant method

* Avoid calculation of Jacobian exactly at every iteration

* Approximate Jacobian (or its inverse) is updated with easier steps at every iteration.

* Convergence rate is superlinear

To solve

$$\bar{F}(\bar{x}) = 0 \qquad \text{———} \ (1)$$

$$\bar{F} = [f_1 \ f_2 \ \cdots \ f_n]^T \ / \ (f_1, \cdots, f_n)$$

$$\bar{x} = [x_1 \ x_2 \ \cdots \ x_n] \ / \ (x_1, \cdots, x_n)$$

Newton's method:

$$\bar{x}^{(k+1)} = \bar{x}^{(k)} - J^{(k)^{-1}} F(\bar{x}^{(k)}) \qquad \text{———} \ (2)$$

In one dimension,

$$f'(x_{k}) \approx \frac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}} \quad \checkmark$$

$$\underline{\underline{J^{(k)}}} \approx \frac{F(\bar{x}^{(k)}) - F(\bar{x}^{(k-1)})}{\bar{x}^{(k)} - \bar{x}^{(k-1)}}$$

→ Division by a vector!

$$J^{(k)} \Delta \bar{x}^{(k-1)} \approx \Delta F^{(k-1)}$$

We try to find approximate Jacobian, say A_k such that

$$A_k\left(\bar{x}^{(k)} - \bar{x}^{(k-1)}\right) = F(\bar{x}^{(k)}) - F(\bar{x}^{(k-1)}) \quad \text{—— (3)}$$

(3) is known as secant condition.

$$\begin{cases} \Delta \bar{x}^{(k-1)} = \bar{x}^{(k)} - \bar{x}^{(k-1)} \\ \Delta \bar{F}^{(k-1)} = F(\bar{x}^{(k)}) - F(\bar{x}^{(k-1)}) \end{cases}$$

(3) $\Rightarrow$ $$A_k \,\Delta \bar{x}^{(k-1)} = \Delta \bar{F}^{(k-1)} \quad \text{—— (4)}$$

In Broyden's method, find A_{k+1} using A_k as follows

$\longrightarrow$ $$A_{k+1} = A_k + U_k \quad \text{—— (5)}$$

where $U_k = \bar{a}_k \bar{b}_k^T$ (Rank one matrix)

WKT $\bar{x}^{(k+1)}$ (in Newton's method) is the root (soln) of the linear eqn

$$h_k(x) = \bar{F}(\bar{x}^{(k)}) + J^{(k)}(\bar{x} - \bar{x}^{(k)}) \quad \text{—— (6)}$$

ie, $h_k(\bar{x}^{(k+1)}) = 0$. Replace $J^{(k)}$ with approximation A_k

$$l_k(\bar{x}) = F(\bar{x}^{(k)}) + A_k(\bar{x} - \bar{x}^{(k)}) \quad \text{—— (7)}$$

Secant condition at $(k+1)^{th}$ iteration

$$A_{k+1}(\bar{x}^{(k+1)} - \bar{x}^{(k)}) = \bar{F}^{(k+1)} - \bar{F}^{(k)}$$

$$A_{k+1}\, \Delta \bar{x}^{(k)} = \Delta \bar{F}^{(k)} \quad \text{———} \quad (8)$$

Use (5) in (8),

$$(A_k + \bar{a}_k \bar{b}_k^T)\, \Delta \bar{x}^{(k)} = \Delta \bar{F}^{(k)}$$

$$A_k \Delta \bar{x}^{(k)} + (\bar{a}_k \underbrace{\bar{b}_k^T)\, \Delta \bar{x}^{(k)}} = \Delta \bar{F}^{(k)}$$

$$A_k \Delta \bar{x}^{(k)} + (\bar{b}_k^T \Delta \bar{x}^{(k)})\, \bar{a}_k = \Delta \bar{F}^{(k)}$$

$$\bar{a}_k = \frac{\Delta \bar{F}^{(k)} - A_k \Delta \bar{x}^{(k)}}{\bar{b}_k^T \Delta \bar{x}^{(k)}} \quad \text{———} \quad (9)$$

$$l_{k+1}(\bar{x}) - l_k(\bar{x}) = \bar{F}^{(k+1)} + A_{k+1}(\bar{x} - \bar{x}^{(k+1)}) - \{\bar{F}^{(k)} + A_k(\bar{x} - \bar{x}^{(k)})\}$$

$$= \Delta \bar{F}^{(k)} + A_{k+1}(\underbrace{\bar{x} - \bar{x}^{(k)}}_{c} + \underbrace{\bar{x}^{(k)} - \bar{x}^{(k+1)}}) - A_k(\underbrace{\bar{x} - \bar{x}^{(k)}}_{c})$$

$$= \underbrace{\Delta \bar{F}^{(k)} - A_{k+1}(\Delta \bar{x}^{(k)})}_{\text{zero secant condi.}} + \underbrace{(A_{k+1} - A_k)}_{\bar{a}_k \bar{b}_k^T}(\bar{x} - \bar{x}^{(k)})$$

$$\underline{l_{k+1}(\bar{x}) - l_k(\bar{x})} = \bar{a}_k \bar{b}_k^T (\bar{x} - \bar{x}^{(k)})$$

$$= \{\bar{b}_k^T (\bar{x} - \bar{x}^{(k)})\}\, \bar{a}_k \quad \text{———} \quad (10)$$

Enforce $l_{k+1}(\bar{x}) - l_k(\bar{x}) = 0$

$$\Rightarrow \{\bar{b}_k^T (\bar{x} - \bar{x}^{(k)})\}\, \bar{a}_k = 0$$

$$\Rightarrow \text{either } \bar{a}_k = \bar{0} \text{ or } \bar{b}_k \perp (\bar{x} - \bar{x}^{(k)})$$

$l_k(\bar{x}^{(k+1)}) = 0$

$l_{k+1}(\bar{x}^{(k+1)}) = \bar{F}(\bar{x}^{(k+1)})$

$$A_k \Delta \bar{x}^{(k+1)} = \Delta F^{(k+1)}$$

If $\bar{a}_k = 0 \Rightarrow A_k \Delta \bar{x}^{(k)} = \Delta F^{(k)}$

$\Rightarrow$ Secant condition for the next step is also satisfied by A_k, which is not desireable.

$$\bar{b}_k' \perp (\bar{x} - \bar{x}^{(k)})$$

Choose $\bar{b}_k = \bar{x}^{(k+1)} - \bar{x}^{(k)} = \Delta \bar{x}^{(k)}$

(In Broyden's method)

i.e, $(\bar{x} - \bar{x}^{(k+1)}) \perp \Delta \bar{x}^{(k)}$

$$\bar{b}_k = \Delta \bar{x}^{(k)} \quad \text{— 11} \qquad \bar{a}_k = \frac{\Delta \bar{F}^{(k)} - A_k \Delta \bar{x}^{(k)}}{\Delta \bar{x}^{(k)T} \Delta \bar{x}^{(k)}}$$

$$= \frac{\Delta \bar{F}^{(k)} - A_k \Delta \bar{x}^{(k)}}{\| \Delta \bar{x}^{(k)} \|_2^2} \quad \text{— 12}$$

$$A_{k+1} = A_k + \bar{a}_k \bar{b}_k^T$$

Algorithm

$\bar{x}^{(0)}$ $\bar{F}$

Find $\bar{F}^{(0)}$, $\bar{J}^{(0)} = A_0$

For $k = 0, 1, \ldots$ solve $A_k \bar{h}_k = \bar{F}^{(k)}$

$\bar{x}^{(k+1)} = \bar{x}^{(k)} - \underbrace{A_k^{-1} \bar{F}^{(k)}}_{h_k}$

Evaluate $\bar{F}^{(k+1)}$

$\Delta \bar{F}^{(k)} = \bar{F}^{(k+1)} - \bar{F}^{(k)}$

$b_k = \bar{x}^{(k+1)} - \bar{x}^{(k)}$

$\bar{c} = \Delta F^{(k)} - A_k \bar{b}_k$

$\alpha = \bar{b}_k^T \bar{b}_k$

$a_k = \bar{c}/\alpha$

$A_{k+1} = A_k + \bar{a}_k \bar{b}_k^T$

end

For large no: of vari:bls do not go for direct inverse

$\bar{x}^{(1)} = \bar{x}^{(0)} + \bar{h}^{(0)}$

$A_0 \bar{h}^{(0)} = -\bar{F}^{(0)}$

$$\boxed{\bar{F}(\bar{x}) = \bar{0}}$$

$\bar{x} = (x_1, x_2, x_3)$ $\quad \bar{F} = (f_1, f_2, f_3)$

Exe $\quad \bar{F}(\bar{x}) = \left(\underline{x_1^2 + x_2^2 + x_3^2 - 3}, \; \underline{x_1^2 + x_2^2 - x_3 - 1}, \; \underline{x_1 + x_2 + x_3 - 3} \right)$

$$\bar{x}^{(0)} = (1, 0, 1)$$

Need to provide $\quad A_0 = J(\bar{x}^{(0)}) \quad \& \quad \bar{x}^{(1)} = \bar{x}^{(0)} + \bar{h}^{(0)}$

$$J(\bar{x}) = \begin{bmatrix} 2x_1 & 2x_2 & 2x_3 \\ 2x_1 & 2x_2 & -1 \\ 1 & 1 & 1 \end{bmatrix} \qquad \bar{F}(\bar{x}) = \begin{bmatrix} x_1^2 + x_2^2 + x_3^2 - 3 \\ x_1^2 + x_2^2 - x_3 - 1 \\ x_1 + x_2 + x_3 - 3 \end{bmatrix}$$

$$A_0 = \bar{J}^{(0)} = \begin{bmatrix} 2 & 0 & 2 \\ 2 & 0 & -1 \\ 1 & 1 & 1 \end{bmatrix} \qquad \bar{F}^{(0)} = \begin{bmatrix} -1 \\ -1 \\ -1 \end{bmatrix}$$

$$A_0 \bar{h}^{(0)} = -\bar{F}^{(0)}$$

$$\begin{bmatrix} 2 & 0 & 2 \\ 2 & 0 & -1 \\ 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} h_1^{(0)} \\ h_2^{(0)} \\ h_3^{(0)} \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \longrightarrow \text{Use Gauss Elimination}$$

HW

$$\Longrightarrow \quad \bar{h}^{(0)} = \begin{bmatrix} h_1^{(0)} \\ h_2^{(0)} \\ h_3^{(0)} \end{bmatrix} = \begin{bmatrix} 1/2 \\ 1/2 \\ 0 \end{bmatrix}$$

$$\bar{x}^{(2)} = \begin{bmatrix} 5/4 \\ 3/4 \\ 1 \end{bmatrix} \qquad \bar{x}^{(1)} = \bar{x}^{(0)} + \bar{h}^{(0)} = \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} + \begin{bmatrix} 1/2 \\ 1/2 \\ 0 \end{bmatrix} = \begin{bmatrix} 3/2 \\ 1/2 \\ 1 \end{bmatrix}$$

$$\bar{b}_0 = \Delta \bar{x}^{(0)}, \quad \Delta \bar{F}^{(0)} \quad \bar{a}_0 \bar{b}_0^T = \underbrace{\frac{[\Delta F^{(0)} - A_0 b_0]\, \bar{b}_0^T}{\bar{b}_0^T \bar{b}_0}}_{\bar{a}_0^T}$$

$$\bar{x}^{(0)} = \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} \qquad \bar{x}^{(1)} = \begin{bmatrix} 3/2 \\ 1/2 \\ 1 \end{bmatrix},$$

$$\bar{h}^{(0)} = \begin{bmatrix} 1/2 \\ 1/2 \\ 0 \end{bmatrix} = \Delta \bar{x}^{(0)} = \bar{b}_0$$

$$F(\bar{x}^{(0)}) = \bar{F}^{(0)} = \begin{bmatrix} -1 \\ -1 \\ -1 \end{bmatrix} \qquad \bar{F}^{(1)} = \begin{bmatrix} 1/2 \\ 1/2 \\ 0 \end{bmatrix}$$

$$\Delta \bar{F}^{(0)} = \begin{bmatrix} 3/2 \\ 3/2 \\ 1 \end{bmatrix}$$

$$\bar{a}_0 = \frac{\left(\Delta \bar{F}^{(0)} - A_0 \bar{b}_0\right)}{\bar{b}_0^T \bar{b}_0}$$

$$A_0 \bar{b}_0 = \begin{bmatrix} 2 & 0 & 2 \\ 2 & 0 & -1 \\ 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1/2 \\ 1/2 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

$$\bar{a}_0 = \frac{\begin{bmatrix} 3/2 \\ 3/2 \\ 1 \end{bmatrix} - \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}}{\begin{bmatrix} 1/2 & 1/2 & 0 \end{bmatrix} \begin{bmatrix} 1/2 \\ 1/2 \\ 0 \end{bmatrix}}$$

$$= 2 \left\{ \begin{bmatrix} 1/2 \\ 1/2 \\ 0 \end{bmatrix} \right\} = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}$$

$$A_1 = A_0 + a_0 b_0^T$$

$$= \begin{bmatrix} 2 & 0 & 2 \\ 2 & 0 & -1 \\ 1 & 1 & 1 \end{bmatrix} + \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} \begin{bmatrix} 1/2 & 1/2 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} & & \\ & & \\ & & \end{bmatrix} + \begin{bmatrix} 1/2 & 1/2 & 0 \\ 1/2 & 1/2 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} 5/2 & 1/2 & 2 \\ 5/2 & 1/2 & -1 \\ 1 & 1 & 1 \end{bmatrix}$$

Find $\Delta \bar{x}^{(1)} = \bar{h}^{(1)} = \bar{b}_1$

$$A_1 \Delta \bar{x}^{(1)} = -\bar{F}^{(1)}$$

$$\begin{bmatrix} 5/2 & 1/2 & 2 \\ 5/2 & 1/2 & -1 \\ 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} \Delta x_1^{(1)} \\ \Delta x_2^{(1)} \\ \Delta x_3^{(1)} \end{bmatrix} = \begin{bmatrix} -1/2 \\ -1/2 \\ 0 \end{bmatrix}$$

G.E

$$\left[\begin{array}{ccc|c} 5/2 & 1/2 & 2 & -1/2 \\ 5/2 & 1/2 & -1 & -1/2 \\ 1 & 1 & 1 & 0 \end{array}\right]$$

$R_2 \to R_2 - R_1$

$\sim$

$R_3 \to R_3 - \frac{2}{5} R_1$

$$\left[\begin{array}{ccc|c} 5/2 & 1/2 & 2 & -1/2 \\ 0 & 0 & -3 & 0 \\ 0 & 4/5 & 1/5 & 1/5 \end{array}\right]$$

$$\sim \left[\begin{array}{ccc|c} 5/2 & 1/2 & 2 & -1/2 \\ 0 & 4/5 & 1/5 & 1/5 \\ 0 & 0 & -3 & 0 \end{array}\right]$$

$$-3\,\Delta x_3^{(1)} = 0 \implies \Delta x_3^{(1)} = 0$$

$$\tfrac{4}{5}\Delta x_2^{(1)} + \tfrac{1}{5}\Delta x_3^{(1)} = \tfrac{1}{5} \implies \Delta x_2^{(1)} = \tfrac{1}{4}$$

$$\tfrac{5}{2}\Delta x_1^{(1)} + \tfrac{1}{2}\times\tfrac{1}{4} + 2\times 0 = -\tfrac{1}{2}$$

$$\Delta x_1^{(1)} = \left(-\tfrac{4}{8} - \tfrac{1}{8}\right)\tfrac{2}{5} = \tfrac{-5}{8}\times\tfrac{2}{5}$$

$$= -\tfrac{1}{4}$$

$$\Delta \bar{x}^{(1)} = \begin{bmatrix} -1/4 \\ 1/4 \\ 0 \end{bmatrix}$$

$$\bar{x}^{(2)} = \bar{x}^{(1)} + \Delta \bar{x}^{(1)}$$

$$= \begin{bmatrix} 3/2 \\ 1/2 \\ 1 \end{bmatrix} + \begin{bmatrix} -1/4 \\ 1/4 \\ 0 \end{bmatrix}$$

$$\bar{x}^{(2)} = \begin{bmatrix} 5/4 \\ 3/4 \\ 1 \end{bmatrix}$$

Theorem (Sherman-Morrison Formula)

Suppose A is a non-singular matrix and let $\bar{a}$ & $\bar{b}$ are vectors with $\bar{b}^T A^{-1} \bar{a} \neq -1$. Then $A + \bar{a}\bar{b}^T$ is non-singular and

$$\boxed{(A + \bar{a}\bar{b}^T)^{-1} = A^{-1} - \frac{A^{-1}(\bar{a}\bar{b}^T)A^{-1}}{1 + \bar{b}^T A^{-1} \bar{a}}}$$

Exc

Taking $A = A_k$

$$\bar{a}_k = \left(\Delta F^{(k)} - A_k \bar{b}_k\right) / \bar{b}_k^T \bar{b}_k$$

$$\bar{b}_k = \Delta \bar{x}^{(k)}$$

S-T

$$A_{k+1}^{-1} = A_k^{-1} + \frac{\left(\bar{b}_k - \overbrace{A_k^{-1} \Delta F^{(k)}}^{\bar{c}}\right) \overbrace{\bar{b}_k^T A_k^{-1}}^{\bar{d}}}{\underbrace{\left(\bar{b}_k^T A_k^{-1} \Delta F^{(k)}\right)}_{\alpha}}$$

$$= A_k^{-1} + \frac{(\bar{b}_k - \bar{c})\,\bar{d}}{\alpha}$$

Consider previous eg:

$$\bar{x}^{(0)} = \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} \qquad \bar{x}^{(1)} = \begin{bmatrix} 1.5 \\ 0.5 \\ 1 \end{bmatrix}$$

$$\bar{b}_0 \equiv \Delta \bar{x}^{(0)} = \begin{bmatrix} 0.5 \\ 0.5 \\ 0 \end{bmatrix} \qquad \Delta \bar{F}^{(0)} = \begin{bmatrix} 1.5 \\ 1.5 \\ 1 \end{bmatrix}$$

$$A_0^{-1} = J_0^{-1} = \begin{bmatrix} 0.1667 & 0.3333 & 0 \\ -0.5 & 0 & 1 \\ 0.3333 & -0.3333 & 0 \end{bmatrix}$$

$$\begin{bmatrix} 1/6 & 1/3 & 0 \\ -1/2 & 0 & 1 \\ 1/3 & -1/3 & 0 \end{bmatrix}$$

$$A_1^{-1} = A_0^{-1} + \frac{\left(\bar{b}_0 - A_0^{-1} \Delta \bar{F}^{(0)}\right) \bar{b}_0^T A_0^{-1}}{\bar{b}_0^T A_0^{-1} \Delta \bar{F}^{(0)}}$$

$$\bar{c} = A_0^{-1} \Delta \bar{F}^{(0)} \qquad \bar{c} = \begin{bmatrix} 3/4 \\ 1/4 \\ 0 \end{bmatrix}$$

$$\alpha = \bar{b}_0^T \bar{c} \qquad \alpha = 1/2$$

$$\bar{d} = \bar{b}_0^T A_0^{-1}$$

$$\bar{d} = \begin{bmatrix} 1/2 & 1/2 & 0 \end{bmatrix} \begin{bmatrix} 1/6 & 1/3 & 0 \\ -1/2 & 0 & 1 \\ 1/3 & -1/3 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} -1/6 & 1/6 & 1/2 \end{bmatrix}$$

$$\bar{b}_0 - \bar{c} = \begin{bmatrix} 1/2 \\ 1/2 \\ 0 \end{bmatrix} - \begin{bmatrix} 3/4 \\ 1/4 \\ 0 \end{bmatrix} = \begin{bmatrix} -1/4 \\ 1/4 \\ 0 \end{bmatrix}$$

$$A_1^{-1} = A_0^{-1} + \frac{(\bar{b}_0 - \bar{c})\,\bar{d}}{\alpha}$$

$$= \begin{bmatrix} 1/6 & 1/3 & 0 \\ -1/2 & 0 & 1 \\ 1/3 & -1/3 & 0 \end{bmatrix} + \frac{\begin{bmatrix} -1/4 \\ 1/4 \\ 0 \end{bmatrix} \begin{bmatrix} -1/6 & 1/6 & 1/2 \end{bmatrix}}{1/2}$$

$$A_1^{-1} = \begin{bmatrix} 1/4 & 1/4 & -1/4 \\ -7/12 & 1/12 & 5/4 \\ 1/3 & -1/3 & 0 \end{bmatrix} \qquad \begin{bmatrix} 1/2 \\ 1/2 \\ 0 \end{bmatrix}$$

$$\Delta \bar{x}^{(1)} = -A_1^{-1} \bar{F}^{(1)} = \begin{bmatrix} -1/4 \\ 1/4 \\ 0 \end{bmatrix} \quad ? \checkmark$$

$$\bar{x}^{(2)} = \bar{x}^{(1)} + \Delta \bar{x}^{(1)} = \begin{bmatrix} 5/4 \\ 3/4 \\ 1 \end{bmatrix}$$

27/2/24 35, 16, 26, 7

29/2/24 32

Numerical Differentiation & Integration

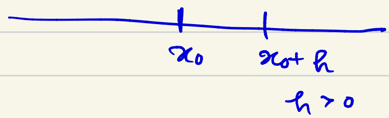
Differentiation

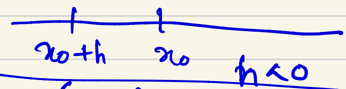
$x_0 \in [a,b]$ & $f \in C^2[a,b]$

$$f'(x_0) = \lim_{h \to 0} \frac{f(x_0+h) - f(x_0)}{h} \qquad (1)$$

Approximate formulae for $f'(x_0)$

$$f'(x_0) \approx \frac{f(x_0+h) - f(x_0)}{h}$$





$h>0$ Order of accuracy (order of error)

first order $O(h)$

second order $O(h^2)$

$h \to$ 0.5 0.2 0.1 0.01

At $h=0.5$ $O(h^2)$ formula is expected to give more accurate soln than $O(h)$ formula.

Lagrange Interpolation formula

$x_0, x_1, x_2, \dots, x_n$ $\quad$ $(n+1)$ points equally spaced

$$x_i - x_{i-1} = h \qquad i = 1, 2 \dots n$$

$\to (x_0, f(x_0)) \; (x_1, f(x_1)) \; \dots \; (x_n, f(x_n))$

$$f(x) \simeq P_n(x) = f(x_0) L_0(x) + f(x_1) L_1(x) + \dots + f(x_n) L_n(x) \quad (2)$$

$$f(x) = P_n(x) + \underbrace{\left[\prod_{i=0}^{n} (x - x_i) \right] \frac{f^{(n+1)}(\xi(x))}{(n+1)!}}_{E_n(x)} \quad (3)$$

$f \in C^{n+1}[a,b]$, where $x_i \in [a,b]$

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

Let $n = 1$ $\qquad x_0, x_1 \qquad x_1 = x_0 + h$

$$f(x) = f(x_0) L_0(x) + f(x_1) L_1(x) + (x-x_0)(x-x_1) \times \frac{f''(\xi(x))}{2!}$$

$$f(x) = f(x_0) \frac{(x - x_1)}{(x_0 - x_1)} + f(x_1) \frac{(x - x_0)}{(x_1 - x_0)} + (x-x_0)(x-x_1) \frac{f''(\xi(x))}{2!} \quad (4)$$

$$f(x) = f(x_0)\frac{(x-x_0-h)}{-h} + f(x_0+h)\frac{(x-x_0)}{h} + (x-x_0)(x-x_0-h)\frac{f''(\xi(x))}{2!}$$

$$f'(x) = \frac{f(x_0)}{-h}\times 1 + \frac{f(x_0+h)}{h}\times 1 + \frac{d}{dx}\{(x-x_0)(x-x_0-h)\}\times\frac{f''(\xi(x))}{2!} + (x-x_0)(x-x_0-h)\frac{d}{dx}\left(\frac{f''(\xi(x))}{2!}\right)$$

$\xi(x)$

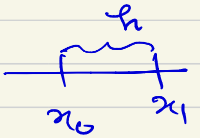
$$f'(x) = \frac{f(x_0+h)-f(x_0)}{h} + \left(\frac{2(x-x_0)-h}{2!}\right)f''(\xi(x)) + \frac{(x-x_0)(x-x_0-h)}{2}\frac{d}{dx}\left(f''(\xi(x))\right)$$

Put $x = x_0$ in above formula

$$f'(x_0) = \frac{f(x_0+h)-f(x_0)}{h} - \underbrace{\frac{f''(\xi_0)}{2!}h}_{\text{error.}}$$

First order formula $(O(h))$

$$f'(x_0) \approx \frac{f(x_0+h)-f(x_0)}{h}$$



$$f'(x_1) \approx \frac{f(x_1)-f(x_1-h)}{h}$$

$O(h)$

$$\pm\frac{f''(\xi_1)}{2!}h$$

$$\left\{ \begin{array}{l} f'(x_0) \simeq \dfrac{f(x_0+h) - f(x_0)}{h} \\ f'(x_0) \simeq \dfrac{f(x_0) - f(x_0-h)}{h} \end{array} \right\}$$

first order

→ derived at x_1 from interpol. formula

x_0, x_1, x_2

$$f(x) = f(x_0) L_0(x) + f(x_1) L_1(x) + f(x_2) L_2(x) + \prod_{i=0}^{2} (x - x_i) \frac{f'''(\xi(x))}{3!}$$

$$L_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} = \frac{(x-x_1)(x-x_2)}{2h^2}$$

$$L_1(x) = \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} = \frac{(x-x_0)(x-x_2)}{-h^2}$$

$$L_2(x) = \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} = \frac{(x-x_0)(x-x_1)}{2h^2}$$

$$f'(x) = f(x_0) \underline{L_0'(x)} + f(x_1) \underline{L_1'(x)} + f(x_2) \underline{L_2'(x)}$$

$$+ \frac{d}{dx} \left\{ (x-x_0)(x-x_1)(x-x_2) \right\} \frac{f'''(\xi(x))}{3!}$$

$$+ (x-x_0)(x-x_1)(x-x_2) \frac{d}{dx} \left(\frac{f'''(\xi(x))}{3!} \right)$$

$$\underline{L_0'(x)} = \frac{2x - x_1 - x_2}{2h^2} \qquad \underline{L_1'(x)} = \frac{2x - x_0 - x_2}{-h^2}$$

$$L_2'(x) = \frac{2x - x_0 - x_1}{2h^2}$$

$$f'(x) = f(x_0)\left[\frac{2x - x_1 - x_2}{2h^2}\right] + f(x_1)\left[\frac{2x - x_0 - x_2}{-h^2}\right] + f(x_2)\left[\frac{2x - x_0 - x_1}{2h^2}\right]$$

$$+ \frac{d}{dx}\left\{(x-x_0)(x-x_1)(x-x_2)\right\}\frac{f'''(\xi(x))}{3!} + (x-x_0)(x-x_1)(x-x_2)\frac{d}{dx}\left(\frac{f'''(\xi(x))}{3!}\right)$$

(x_0, x_1, x_2)

Complete.

$x_0, \quad x_0 + h = x_1, \quad x_0 + 2h = x_2$

$x = x_0$

$\xi(x) = \xi_0$

$$f'(x_0) = \frac{1}{2h}\left[-3f(x_0) + 4f(x_1) - f(x_2)\right] + \frac{h^2}{3} f^{(3)}(\xi_0)$$

$x = x_1$

$\xi(x) = \xi_1$

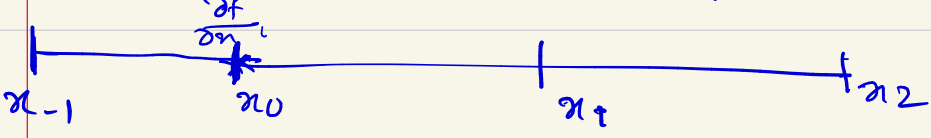
$$f'(x_1) = \frac{1}{2h}\left[f(x_2) - f(x_0)\right] - \frac{h^2}{6} f^{(3)}(\xi_1)$$

$x = x_2$

$\xi(x) = \xi_1$

$$f'(x_2) = \frac{1}{2h}\left[f(x_0) - 4f(x_1) + 3f(x_2)\right] + \frac{h^2}{3} f^{(3)}(\xi_2)$$

2^{nd} order accurate formulae



$$f''(x_0) = \frac{f(x_0+h) - 2f(x_0) + f(x_0-h)}{h^2}$$

$\because$ can derive $x = x_0 + h)$

① $$f(x_0+h) = f(x_0) + hf'(x_0) + \frac{h^2}{2!}f''(x_0) + \frac{h^3}{3!}f^{(3)}(x_0) + \boxed{\frac{h^4}{4!}f^{(4)}(\xi(x))}$$

$$\text{error term} = \frac{h^3}{3!}f^{(3)}(\xi(x)) = \frac{h^3}{3!}f^{(3)}(x_0) + \frac{h^4}{4!}f^{(4)}(x_0) + \cdots \quad \text{error term}$$

$$f'(x_0) = \frac{f(x_0+h) - f(x_0)}{h} - \frac{h}{2!}f''(\xi_0)$$

② $$f(x_0-h) = f(x_0) - hf'(x_0) + \frac{h^2}{2!}f''(x_0) - \frac{h^3}{3!}f^{(3)}(x_0) + \boxed{\frac{h^4}{4!}f^{(4)}(\eta(x))}$$

$$\frac{h^2}{2!}f(\eta(x))$$

$$f'(x_0) = \frac{f(x_0) - f(x_0 \ldots)}{h} + \frac{}{2!}f(\eta_0)$$

① + ②

$$f(x_0+h) + f(x_0-h) = 2f(x_0) + 2 \times \frac{h^2}{2!}\boxed{f''(x_0)} + \frac{h^4}{3!}\left(f^{(4)}(\xi(x)) + f^{(4)}(\eta(x))\right)$$

$$f''(x_0) = \frac{f(x_0+h) - 2f(x_0) + f(x_0-h)}{h^2} - \frac{h^2}{4!}f^{(4)}(\gamma_0)$$

$$\frac{h^4}{4!}f^{(4)}(\gamma(x))$$

$\boxed{f \in C^3[a,b] \quad x_0 \in (a,b)}$

$$f''(x_0) \approx \frac{f(x_0+h) - 2f(x_0) + f(x_0-h)}{h^2}$$

Exc

$$f(x) = e^{x^2} \qquad f'(x) = 2x e^{x^2}$$

$$f''(x) = 2e^{x^2} + 2x \times 2x e^{x^2}$$
$$= (4x^2 + 2) e^{x^2}$$

Calculate $f'(1)$ & $f''(1)$ using both first order & 2^{nd} order formulae.

$h = 0.1$

0.8 0.9 1 1.1 1.2

Calculate $f'(1)$

Calculate absolute & relative errors w.r.t exact value

Exact $\quad f'(1) = 2e = 5.4366$

fwd diff (1st order) $\quad f'(1) \approx \dfrac{f(1+0.1) - f(1)}{0.1} = 6.3520$

1 1.1

cent diff (2nd ord) $\quad f'(1) \approx \dfrac{\overset{f(1.1)}{f(1+0.1)} - \overset{f(0.9)}{f(1-0.1)}}{2 \times 0.1} = 5.5279$ ✓

0.9 1 1.1

fwd diff (2nd ord) $\quad f'(1) \approx \dfrac{1}{2 \times 0.1}\left[-3 \times f(1) + 4\,\overset{f(1.1)}{f(1+0.1)} - \overset{f(1.2)}{f(1+0.2)}\right]$ ✓

1 1.1 1.2

$= 5.1919$

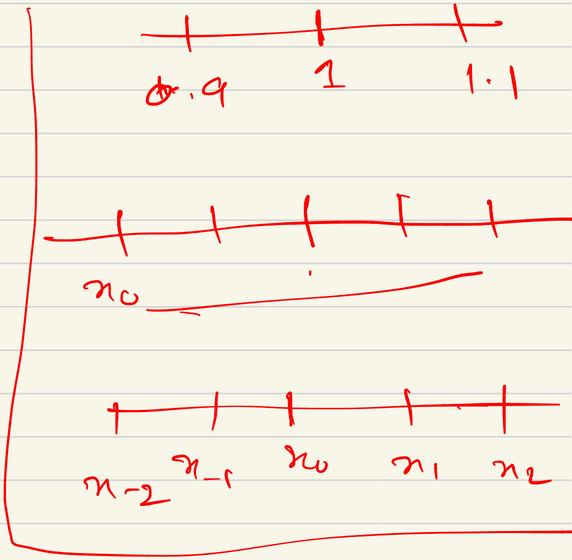
$$f''(1) = 16.3097$$

2nd order central diff

$$f''(1) \approx \frac{f(1+0.1) - 2f(1) + f(1-0.1)}{(0.1)^2}$$

$$= 16.4829$$

$h \longrightarrow 0$



Numerical Integration

- $*$ Trapezoidal & Simpson's rules. ✓
- $*$ 2-D
- $*$ Adaptive - Simpson's
- → $*$ Gauss quadrature rules (Legendre poly)
- → $*$ Monte-Carlo integration method

I Trapezoidal & Simpson's rules

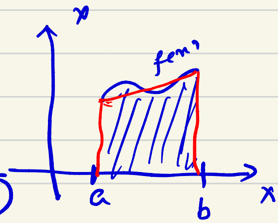
$$\int_a^b f(x)\,dx$$

Lagrange Interpolation $f(x) \approx \sum_{j=0}^{n} f(x_j)\, L_j(x)$ ——— ①

$n=1 \quad x_0 = a \quad x_1 = b$

$$f(x) \approx f(x_0) L_0(x) + f(x_1) L_1(x)$$

$$= f(x_0)\frac{(x-x_1)}{(x_0-x_1)} + f(x_1)\frac{(x-x_0)}{(x_1-x_0)}$$



$$= f(a)\frac{(x-b)}{(a-b)} + f(b)\frac{(x-a)}{(b-a)}$$

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

$$= \frac{f(a)}{-(b-a)}\left(\frac{x^2}{2} - bx\right)_a^b + \frac{f(b)}{(b-a)}\left(\frac{x^2}{2} - ax\right)_a^b$$

$$= \frac{f(a)}{-(b-a)}\left(\underbrace{\overbrace{\frac{b^2}{2} - b^2}^{-b^2/2} - \frac{a^2}{2} + ab}\right) \quad a^2/2$$

$$+ \frac{f(b)}{(b-a)}\left(\underbrace{\frac{b^2}{2} - ab - \overbrace{\frac{a^2}{2} + a^2}}\right)$$

②

$$\frac{b-a}{2}\left[f(a) + f(b)\right] = \frac{1}{2\cancel{(b-a)}}\left[+f(a)\,(b-a)^{\cancel{2}} + f(b)\,(b-a)^{\cancel{2}}\right]$$

Trapezoidal rule

$x_i - x_{i-1} = h$

$a = x_0 \quad x_1 \quad x_2 \quad \cdots \quad x_{n-1} \quad x_n = b$

$$\int_a^b f(x)\,dx = \int_{a=x_0}^{x_1} f(x)\,dx + \int_{x_1}^{x_2} f(x)\,dx + \cdots + \int_{x_{n-1}}^{x_n=b} f(x)\,dx$$

$$\approx \frac{h}{2}\left(f(x_0)+f(x_1)\right) + \frac{h}{2}\left(f(x_1)+f(x_2)\right) + \cdots + \frac{h}{2}\left(f(x_{n-1})+f(x_n)\right)$$

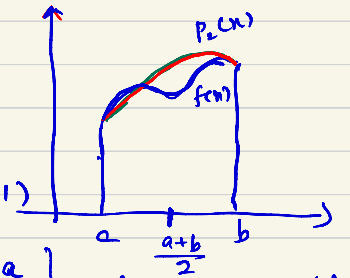
Composite Trapezoidal rule

$$\int_a^b f(x)\,dx \approx \frac{h}{2}\left[f(x_0) + 2\left(f(x_1)+\cdots+f(x_{n-1})\right) + f(x_n)\right] \quad (3)$$

Simpson's 1/3rd rule

$x_0 = a \qquad x_1 = \frac{a+b}{2} \qquad x_2 = b$

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



$$f(x) \approx f(x_0) + \frac{\Delta f(x_0)}{1!}s + \frac{\Delta^2 f(x_0)}{2!}s(s-1) \quad (4)$$

$x = a \Rightarrow s = 0$

$x = b \Rightarrow s = \frac{b-a}{h} = 2$

$s = \frac{x-a}{h}$ $\quad \frac{ds}{dx} = \frac{1}{h} \quad ds = \frac{1}{h}dx$

$$\int_a^b f(x)\,dx \approx \int_a^b \left[f(x_0) + \frac{\Delta f(x_0)}{1!}s + \frac{\Delta^2 f(x_0)}{2!}s(s-1)\right]dx$$

$$= h\int_0^2 \left\{f(x_0) + \Delta f(x_0)\,s + \frac{\Delta^2 f(x_0)}{2!}(s^2 - s)\right\}ds$$

$x_0 \quad x_1$

$\Delta f(x_0) = f(x_0+h) - f(x_0) = f(x_1) - f(x_0)$

$\Delta^2 f(x_0) = f(x_0+2h) - 2f(x_0+h) + f(x_0)$

$$h\left[f(x_0)(s)\Big|_0^2 + \Delta f(x_0)\left(\frac{s^2}{2}\right)\Big|_0^2 + \frac{\Delta^2 f(x_0)}{2!}\left(\frac{s^3}{3} - \frac{s^2}{2}\right)\Big|_0^2\right]$$

$$= h\left[f(x_0)(2) + \left(f(x_1) - f(x_0)\right)(2) + \frac{\left(f(x_2) - 2f(x_1) + f(x_0)\right)}{2!}\left(\frac{8}{3} - 2\right)\right]$$

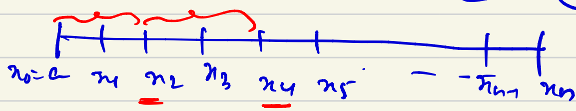
$\frac{8}{3} - 2 = 2/3$

$$= h\left[\frac{1}{3}f(x_0) + \frac{4}{3}f(x_1) + \frac{1}{3}f(x_2)\right]$$

$x_0 = a \quad x_1 = \frac{a+b}{2} \quad x_2 = b$

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

$$\int_a^b f(x)\,dx \approx \frac{h}{3}\left[\underbrace{f(x_0)}_{a} + 4\underbrace{f(x_1)}_{\frac{a+b}{2}} + \underbrace{f(x_2)}_{b}\right] \quad (5)$$



Composite Simpson's $1/3$rd rule

$$\underbrace{\int_{a=x_0}^{b=x_n} f(x)\,dx = \int_{x_0}^{x_2} f(x)\,dx + \int_{x_2}^{x_4} f(x)\,dx + \cdots + \int_{x_{n-2}}^{x_n} f(x)\,dx}_{n \to \text{even}}$$

$$= \frac{h}{3}\left(f(x_0) + 4f(x_1) + f(x_2)\right) + \frac{h}{3}\left(f(x_2) + 4f(x_3) + f(x_4)\right)$$
$$+ \frac{h}{3}\left(f(x_4) + 4f(x_5) + f(x_6)\right) + \cdots$$
$$+ \frac{h}{3}\left(f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)\right)$$

$$\int_a^b f(x)\,dx \approx \frac{h}{3}\left[f(x_0) + 4\sum_{i=1}^{n/2} f(x_{2i-1}) + 2\sum_{i=1}^{n/2-1} f(x_{2i}) + f(x_n)\right] \quad (6)$$

HW

Simpson's $3/8$th rule $\longrightarrow$ divide interval $[a,b]$ into 3 subintervals

$a, \ \frac{2a+b}{3}, \ \frac{a+2b}{3}, \ b$

$x_0 \quad x_1 \quad x_2 \quad x_3$

$x_i - x_{i-1} = \frac{b-a}{3}$

$$f(x) \approx f(x_0) + \Delta f(x_0)\, s + \frac{\Delta^2 f(x_0)}{2!} s(s-1) + \frac{\Delta^3 f(x_0)}{3!} s(s-1)(s-2)$$

$s = \frac{x-a}{h}$

$$\int_a^b f(x)\,dx \approx \frac{3h}{8}\left[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)\right] \quad (7)$$

Eg: Evaluate $\int_4^{5.2} \log_e x \, dx$ using both Trapezoidal & Simpson's 1/3rd rule. Take $n=6$. Compare with exact soln

$a = 4 \quad b = 5.2 \quad n = 6 \quad h = \frac{5.2-4}{6} = 0.2$

$\log_e x$

x_i	4	4.2	4.4	4.6	4.8	5	5.2
$f(x_i)$	1.38629						

Exact 1.8278

T. Rule
$$\int_4^{5.2} \log_e x \, dx \approx \frac{0.2}{2}\left[\log_e(4) + 2\left(\log_e 4.2 + \log_e 4.6 + \log_e 4.8 + \log_e 5\right) + \log_e 5.2\right]$$

$= 1.827655138$ error 10^{-4} 1.9227×10^{-4}

Simpson's 1/3rd rule
$$\int_4^{5.2} \log_e x \, dx \approx \frac{0.2}{3}\left[\log_e(4) + 4\left(\log_e 4.2 + \log_e 4.6 + \log_e 5\right) + 2\left(\log_e 4.4 + \log_e 4.8\right)\right]$$

$= 1.827847725795$

Exact: 1.827847409 error 10^{-7}

$$\underset{[a,b]}{\text{avg}}\, f = \frac{1}{b-a}\int_a^b f(x)\,dx$$

Error in Trapezoidal rule

Thm 1 Mean value Thm (for integrals)

If f is continuous on $[a,b]$, then there exists some $c \in [a,b]$ so that

$$f(c) = \frac{1}{b-a}\int_a^b f(x)\,dx \qquad \text{--- (1)}$$

Thm 2 Weighted MVT (for integrals)

Let f is conti on $[a,b]$ & w is integrable on $[a,b]$. Also w never changes its sign on $[a,b]$, then $\exists\, c \in [a,b]$ so that

$$\int_a^b w(x) f(x)\,dx = f(c)\int_a^b w(x)\,dx \qquad \text{--- (2)}$$

$$\boxed{f(c) = \frac{\int_a^b w(x) f(x)\,dx}{\int_a^b w(x)\,dx}}$$

Error in Lagrange interpolation formula.

$$f(x) - \sum_{j=0}^{n} f(x_j) L_j(x) = \underbrace{\prod_{j=0}^{n}(x - x_j)}\, \frac{f^{(n+1)}(\xi_x)}{(n+1)!} \qquad \text{--- (3)}$$

Error in Basic Trapezoidal rule:

$$E = \underbrace{\int_a^b f(x)\,dx - \frac{b-a}{2}\left[f(a) + f(b)\right]}$$

$n = 1$

f is 2 times continuously diff' in $[a,b]$

$$= \int_a^b \underbrace{\left(f(x) - \left[f(x_0)\frac{(x-b)}{(a-b)} + f(x_1)\frac{(x-a)}{(b-a)}\right]\right)}\,dx$$

$$= \int_a^b \left((x-a)(x-b)\,\frac{f^{(2)}(\xi_x)}{2!}\right) dx$$

$$E = \int_a^b \underbrace{(x-a)(x-b)}_{w(x)} \underbrace{\frac{f^{(2)}(\xi_x)}{2!}}_{f(x)} \qquad a < \xi_x < b$$

$$= \frac{f^{(2)}(\xi)}{2!} \int_a^b (x-a)(x-b)\,dx \qquad \xi$$

(By weighted MVT)

$$= \frac{f^{(2)}(\xi)}{2!} \left[(x-a)\frac{(x-b)^2}{2} - \frac{(x-b)^3}{3\times 2} \right]_a^b$$

$$= \frac{f^{(2)}(\xi)}{2!} \left[0 - 0 - 0 + \frac{(a-b)^3}{6} \right]$$

$$E = -\frac{f^{(2)}(\xi)}{12}(b-a)^3 \quad \text{——— (4)}$$

Error in composite Trapezoidal rule.

$x_0, x_1, \ldots x_n \qquad h$

$$Err = \int_a^b f(x)\,dx - \underbrace{\frac{h}{2}\left[f(x_0) + 2(f(x_1) + \cdots + f(x_{n-1})) + f(x_n)\right]}$$

$$= -\sum_{j=1}^{n} \frac{h^3}{12} f''(\xi_j) \qquad \left(\text{Using (4) in } [x_{j-1}, x_j],\ j=1,2 \ldots n\right)$$

$$Err = -\frac{h^3}{12} \times n \left(\frac{1}{n} \sum_{j=1}^{n} f''(\xi_j) \right) \quad \text{——— (5)}$$

{ Since $f \in C^2[a,b]$, $f^{(2)}$ is conti in $[a,b]$

Hence $\min_{[a,b]} f^{(2)}(x) \le \frac{1}{n} \sum_{j=1}^{n} f''(\xi_j) \le \max_{[a,b]} f^{(2)}(x)$

& $f^{(2)}(x)$ is bounded

ie, $\exists\ \eta \in [a,b]$ so that

$$f^{(2)}(\eta) = \frac{1}{n} \sum_{j=1}^{n} f^{(2)}(\xi_j) \quad \text{——— (6)}$$

$$Err = \frac{-h^3}{12}\,\frac{b-a}{h}\,f^{(2)}(\eta)$$

$$\boxed{Err = \frac{-h^2}{12}(b-a)\,f^{(2)}(\eta)}$$

2^{nd} order error

Simpson's $1/3$rd rule: (quadratic interpolation)

3 pt

$a \quad \frac{a+b}{2} \quad b$

$$E = \frac{-(b-a)^5}{90 \times 2^5} f^{(4)}(\xi), \qquad \xi \in [a,b]$$

Composite $Err = \frac{-h^4}{180}(b-a)\,f^{(4)}(\eta), \qquad \eta \in [a,b]$

Commonly used

Simpsons $3/8$th rule (Cubic interpolation)

$$E = \frac{-(b-a)^5}{3^4 \times 80} f^{(4)}(\xi) \qquad \xi \in [a,b]$$

$$Err = \frac{-h^4}{80}(b-a)\,f^{(4)}(\eta) \qquad \eta \in [a,b]$$

Qn. Given $\int_4^{5.2} \log_e x \, dx$. Find the largest possible error in approximating above integral using Trapezoidal & Simpson's 1/3rd rule; when $n=6$

T. Rule:

Absolute error $= \left| \frac{-h^2}{12}(b-a) f^{(2)}(\eta) \right|$, $\eta \in [a,b]$

$a = 4$
$b = 5.2$
$f(x) = \log x$
$f'(x) = \frac{1}{x}$
$f''(x) = \frac{-1}{x^2}$
$h = 0.2$

$\left| \frac{-1}{x^2} \right| \leq \frac{1}{16}$ in $[4, 5.2]$

$$= \frac{(0.2)^2}{12}(5.2-4) \left| f^{(2)}(\eta) \right|$$

$$\leq \frac{0.04 \times 1.2}{12} \times \frac{1}{16}$$

$$= 2.5 \times 10^{-4}$$

Simpson's Rule.

$$\leq 2.5 \times 10^{-7}$$

① — $\int_a^b f(x)\,dx \approx A_0 f(x_0) + A_1 f(x_1) + \dots + A_n f(x_n)$

$x_0, x_1, \dots x_n \to$ equally spaced

Trapezoidal & Simpson's 1/3rd rule

② — $f(x) \approx \underbrace{f(x_0) L_0(x) + \dots + f(x_n) L_n(x)}_{P_n(x)}$

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

$$A_i(x) = \int_a^b L_i(x)\,dx$$

③ — $$\underbrace{f(x) - p_n(x)}_{\text{error}} = \frac{f^{(n+1)}(\xi_x)}{(n+1)!} \prod_{j=0}^{n} (x - x_j)$$

Assume $f(x) = x^5 + 3x^4 + 2x^2 + 1$ $\quad a = 0 \quad b = 1$

$n = 10 \quad h = \frac{1}{10} = 0.1$

$n = 10$	x_0	x_1	$\dots$	x_{10}
	0	0.1		1

$$\int_0^1 f(x)\,dx = \int_0^1 (x^5 + 3x^4 + 2x^2 + 1)\,dx = \left(\frac{x^6}{6} + \frac{3x^5}{5} + \frac{2x^3}{3} + x\right)_0^1$$

$$= \frac{1}{6} + \frac{3}{5} + \frac{2}{3} + 1 = \frac{73}{30} \approx 2.4333\dots$$

Simpson's rule

$$\int_0^1 f(x)\,dx = \frac{0.1}{3}\Big[f(0) + 4\big(f(0.1) + f(0.3) + f(0.5) + f(0.7) + f(0.9)\big)$$
$$+ 2\big(f(0.2) + f(0.4) + f(0.6) + f(0.8)\big) + f(1)\Big]$$

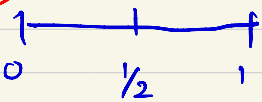
$= 2.4334$

$f(x) = 2x+1$

$$\int_0^1 f(x)\,dx = \int_0^1 (2x+1)\,dx = \left(x^2+x\right)\Big|_0^1$$

$$= 2.$$

$$\int_0^1 f(x)\,dx = \frac{0.5}{3}\left[f(0) + 4f(1/2) + f(1)\right]$$



$$= \frac{1}{6}\left[1 + 4\times 2 + 3\right] = 2$$

Note: If $f(x) = p_n(x)$, then numerical quadrature method that is constructed with n points $x_0, x_1, \dots, x_n$ using (2) will produce exact integral value. i.e.

$$\int_a^b p_n(x)\,dx = A_0\, p_n(x_0) + \cdots + A_n p_n(x_n)$$

where $A_j = \int_a^b l_j(x)\,dx$

In particular, for Simpson's 1/3rd rule provides exact integral value for $f(x) = p_n(x)$, $n \le 2$ & Trapezoidal rule gives exact value if $n \le 1$

Consider $f(x) = \frac{1}{e^x \sqrt{x}}$ $g(x) = \frac{\cos x}{\sqrt{x}}$

$$\int_0^1 \frac{dx}{e^x \sqrt{x}} \quad \text{OR} \quad \int_0^{\pi/2} \frac{\cos x}{\sqrt{x}}\, dx$$

To apply Simpson's rule with $n = 2$

$(x_0 = 0 \quad x_1 = 1/2 \quad x_2 = 1)$

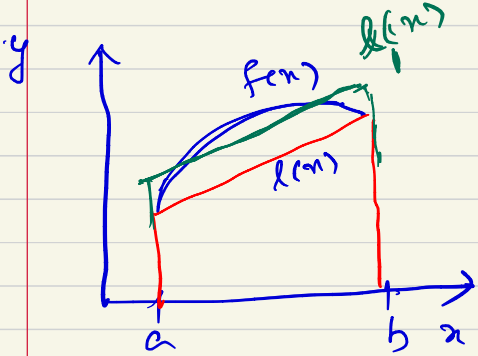
$$\frac{0.5}{3}\left(\underbrace{f(0)}_{\text{not defined}} + 4 f(1/2) + f(1)\right)$$

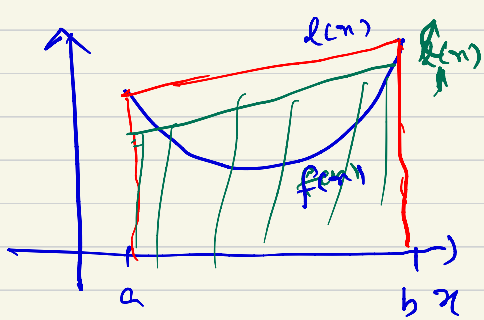
|ly for 2nd integral

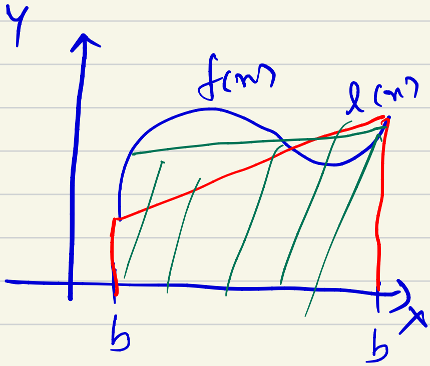
$x = t^2 \qquad dx = 2t\,dt$

$$\int_0^1 \frac{2t\,dt}{e^{t^2}\, t} = \int_0^1 \frac{2\,dt}{e^{t^2}}$$

|ly check for 2nd fn







Eg Determine a quadrature formula of the form $\int_a^b f(x)\,dx \approx \sum_{i=0}^{n} A_i f(x_i)$ for $\int_{-2}^{2} f(x)\,dx$ using the quadratic interpolation at $x_0 = -1$, $x_1 = 0$, $x_2 = 1$

$f(x_0)$ $\quad$ $f(x_1)$ $\quad$ $f(x_2)$

$L_2(x) = \frac{(x+1)x}{2}$

$$f(x) \approx f(x_0)L_0(x) + f(x_1)L_1(x) + f(x_2)L_2(x)$$

$$\int_{-2}^{2} f(x)\,dx \approx f(x_0)\int_{-2}^{2} L_0(x)\,dx + f(x_1)\int_{-2}^{2} L_1(x)\,dx + f(x_2)\int_{-2}^{2} L_2(x)\,dx$$

$$L_0(x) = \frac{x(x-1)}{-1 \times -2} = \frac{x(x-1)}{2}$$

$$L_1(x) = \frac{(x+1)(x-1)}{1 \times -1} = -(x+1)(x-1)$$

$$\underbrace{\int_{-2}^{2} h_0(x)\,dx}_{A_0} = \frac{8}{3}, \quad \underbrace{\int_{-2}^{2} h_1(x)}_{A_1} = \frac{-4}{3}, \quad \underbrace{\int_{-2}^{2} h_2(x)\,dx}_{A_2} = \frac{8}{3}$$

$$\int_{-2}^{2} f(x)\,dx \approx \frac{8}{3} f(-1) - \frac{4}{3} f(0) + \frac{8}{3} f(1)$$

$$= \frac{4}{3}\left[2 f(-1) - f(0) + 2 f(1)\right]$$

$$\frac{b-a}{2} = \frac{4}{2} = 2$$

$-2, 0, 2$

Simpson's $\frac{1}{3}$rd rule

$$\int_{-2}^{2} f(x) \approx \frac{2}{3}\left[f(-2) + 4f(0) + f(2)\right]$$

Theorem: <u>Gauss quadrature theorem</u>

Let p_{n+1} be a non-trivial polynomial of degree $\le n+1$ such that

$$\int_a^b x^k \, p_{n+1}(x)\, dx = 0 \qquad 0 \le k \le n$$

Let $x_0, x_1, \dots x_n$ be the zeroes of p_{n+1}.
Then the formula

$$\int_a^b f(x)\, dx \approx \sum_{i=0}^{n} A_i f(x_i), \quad \text{where}$$

$$A_i = \int_a^b l_i(x)\, dx$$

with these x_i's as nodes will be exact for all polynomials of degree at most $2n+1$.
Furthermore the nodes lie in the open interval (a,b).

$n + (n+1)$

Proof

Let $f(x) = p_{2n+1}(x)$ be a polynomial of degree $\le 2n+1$

Given that p_{n+1} is of degree $\le n+1$

Divide p_{2n+1} by p_{n+1}

$$\frac{p_{2n+1}}{p_{n+1}} = p(x) + \frac{r(x)}{p_{n+1}}$$

$$\Rightarrow \quad p_{2n+1}(x) = p_{n+1}(x)\, p(x) + r(x) \quad \text{——— (1)}$$

Since $p(x)$ is of degree $\le n$

$$\underbrace{\int_a^b p(x)\, p_{n+1}(x)\, dx = 0}_{②} \qquad \left(\text{since } \int_a^b x^k p_{n+1}(x)\,dx = 0 \quad 0 \le k \le n \text{ given condn}\right)$$

Given $x_0, x_1, \ldots x_n$ are zeroes of p_{n+1}

Hence, $\underbrace{P_{2n+1}(x_i) = \underbrace{P_{n+1}(x_i)}_{=0}\, p(x_i) + r(x_i) = r(x_i)}_{③}$

$$\int_a^b P_{2n+1}(x)\, dx = \int_a^b \left[p(x)\, p_{n+1}(x) + r(x)\right] dx$$

$$= \int_a^b r(x)\, dx \quad ④$$

Since $r(x)$ is a poly of degree $\le n$,
if a quadrature formula using interpolation formula using $x_0, x_1 \ldots x_n$ gives you exact formula.

$$\int_a^b p_{2n+1}(x)\,dx = \int_a^b r(x)\, dx = \sum_{i=0}^{n} A_i\, r(x_i)$$

(using ⑥)

$$= \sum_{i=0}^{n} A_i \overbrace{\left(P(x_i)\, \underbrace{p_{n+1}(x_i)}_{0} + r(x_i)\right)}$$

$x_0, x_1, \ldots, x_n$ roots of $p_{n+1}(x) = 0$

$P_{n+1}(x_i) = 0$

$$\boxed{\int_a^b p_{2n+1}(x)\,dx = \sum_{i=0}^{n} A_i\, P_{2n+1}(x_i)}$$

$$= \underbrace{\sum_{i=0}^{n} A_i\, P_{2n+1}(x_i)}_{⑤}$$

$$\int_a^b p_{2n+1}(x)\,dx \quad \int_a^b \left[\underbrace{p(x)\, p_{n+1}(x)} + r(x)\right] dx = \underbrace{\int_a^b r(x)\, dx}_{⑥}$$

Eg: Determine a Gaussian quadrature formula with three Gaussian nodes & three weights for the integral $\int_{-1}^{1} f(x)\,dx$.

We are using 3 Gaussian nodes, say x_0, x_1, x_2.

i.e. According to above thm, construct a 3rd degree poly (3 zeroes!)

$$P_3(x) = c_0 + c_1 x + c_2 x^2 + c_3 x^3 \quad \text{--- (1)}$$

($n+1 = 3$ acc: theorem)

$P_3(x)$ must satisfy,

$$\int_{-1}^{1} P_3(x)\,dx = 0 \qquad \int_{-1}^{1} x\, P_3(x)\,dx = 0 \qquad \int_{-1}^{1} x^2 P_3(x)\,dx = 0 \quad \text{--- (2)}$$

) As a choice let us assume $c_0 = c_2 = 0$

i.e. consider $P_3(x) = c_1 x + c_3 x^3$ --- (3)

This makes $\int_{-1}^{1} P_3(x)\,dx = \int_{-1}^{1} x^2 P_3(x)\,dx = 0$

(already satisfied! No need to enforce)

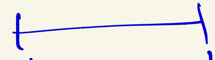
enforcing $\int_{-1}^{1} x\, P_3(x)\,dx = 0 \Rightarrow \int_{-1}^{1} x\,(c_1 x + c_3 x^3)\,dx = 0$

$$\Rightarrow \frac{c_1}{3} + \frac{c_3}{5} = 0 \quad \text{--- (4)}$$

$\hookrightarrow$ Infinite solns.

Choose $c_3 = 5 \Rightarrow c_1 = -3$

Legendre $\approx$ $$P_3(x) = -3x + 5x^3 \quad \text{--- (5)}$$



$-1 \qquad\qquad 1$

$P_3(x) = -3x + 5x^3 = 0$

Roots are : $x(-3+5x^2) = 0 \Rightarrow -\sqrt{3/5},\ 0,\ \sqrt{3/5}$

Gaussian nodes $\longrightarrow$ $x_0 \quad x_1 \quad x_2$

$x_0 = -\sqrt{3/5} \qquad x_1 = 0 \qquad x_2 = \sqrt{3/5}$

Need to construct a formula: (which is exact for poly ≤ 5)

$$\int_{-1}^{1} f(x)\,dx \approx \underline{A_0}\, f(\underbrace{-\sqrt{3/5}}_{x_0}) + \underline{A_1}\, f(\underbrace{0}_{x_1}) + \underline{A_2}\, f(\underbrace{\sqrt{3/5}}_{x_2})$$

One option use interpolation with quadratic poly. $(x_0, f(x_0)),\ (x_1, f(x_1)),\ (x_2, f(x_2))$

$A_0, A_1, A_2 \Rightarrow \int_{-1}^{1} L_0(x)\,dx \quad \int_{-1}^{1} L_2(x)\,dx \quad \int_{-1}^{1} L_3(x)\,dx$

Alternatively use method of undetermined coefficients.

i.e., enforcing the condition that above formula is exact for poly of degree ≤ 2 (three unknowns A_0, A_1, A_2)

The method is exact for poly of degree ≤ 2

$$\int_{-1}^{1} \underbrace{(a_0 + a_1 x + a_2 x^2)}_{f(x)}\,dx = A_0\, f(-\sqrt{3/5}) + A_1 f(0) + A_2\, f(\sqrt{3/5})$$

Basis for poly. of degree ≤ 2

$\{1, x, x^2\} \longrightarrow \{a_0 + a_1 x + a_2 x^2 \,/\, a_i \in \mathbb{R}\}$

Quiz (Theory) — 18^{th} March '24] 15%

Quiz (Pgming) — ~~25^{th}~~ March '24] 10%

$\hookrightarrow 23^{rd}$

$f(x) = 1$

$$\int_{-1}^{1} 1\, dx = A_0 f(-\sqrt{3/5}) + A_1 f(0) + A_2 f(\sqrt{3/5})$$

$$2 = A_0 + A_1 + A_2 \quad \text{—— (1)}$$

$f(x) = x$

$$\int_{-1}^{1} x\, dx = A_0 \times \left(-\sqrt{3/5}\right) + A_1 \times 0 + A_2\left(\sqrt{3/5}\right)$$

$$0 = -\sqrt{3/5}\, A_0 + \sqrt{3/5}\, A_2 \quad \text{—— (2)}$$

$$\int_{-1}^{1} x^2\, dx = A_0 \left(-\sqrt{3/5}\right)^2 + A_1 \times 0^2 + A_2\left(\sqrt{3/5}\right)^2$$

$$\frac{2}{3} = \frac{3}{5} A_0 + \frac{3}{5} A_2 \quad \text{—— (3)}$$

Solve (1) – (3) for A_0, A_1 & A_2

$$A_0 = \frac{5}{9} \qquad A_1 = \frac{8}{9} \qquad A_2 = \frac{5}{9}$$

$$\boxed{\int_{-1}^{1} f(x)\, dx \approx \underbrace{\tfrac{5}{9}}_{w_0} f(\underbrace{-\sqrt{3/5}}_{x_0}) + \underbrace{\tfrac{8}{9}}_{w_1} f(\underbrace{0}_{x_1}) + \underbrace{\tfrac{5}{9}}_{w_2} f(\underbrace{\sqrt{3/5}}_{x_2})}$$

$n = 2$

$\hookrightarrow$ exact for poly degree $\leq 2 \times 2 + 1$

<u>Verification :</u> $\int_{-1}^{1} x^4\,dx = 2\left.\frac{x^5}{5}\right|_0^1 = \frac{2}{5}$

$f(x) = x^4$

$$\int_{-1}^{1} x^4 dx \approx \frac{5}{9}\times\left(-\sqrt{3/5}\right)^4 + \cancel{\frac{8}{9}\times 0}^{\,0} + \frac{5}{9}\left(\sqrt{\frac{3}{5}}\right)^4$$

$$= \frac{2\times 5}{\cancel{9}}\times\frac{\cancel{9}}{25} = \frac{2}{5}$$

Eg → Use above formula to evaluate

$\int_{-1}^{1} e^x \cos x\,dx$. Also compare the solution with Simpson's 1/3rd rule with $n=2$

$f(x) = e^x \cos x$

$$\int_{-1}^{1} e^x \cos x\,dx \approx \frac{5}{9}\left[e^{-\sqrt{3/5}}\cos\left(-\sqrt{3/5}\right)\right] + \frac{8}{9}\left[e^0\cos(0)\right]$$

angle in radians

$$+ \frac{5}{9}\left[e^{\sqrt{3/5}}\cos\left(\sqrt{3/5}\right)\right]$$

$$= 1.933390469 = I_{approx}$$

$$I_{exact} = 1.9334214$$

absolute error $= \left|I_{approx} - I_{exact}\right| = 3.0931\times 10^{-5}$

$h = 1$

Simpsons 1/3rd rule: $(n=2)$ $x_0 = -1,\ x_1 = 0$ $x_2 = 1$

$$\int_{-1}^{1} e^x \cos x\, dx \approx \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right]$$

$$\approx \frac{1}{3}\left[e^{-1}\cos(-1) + 4e^0 \times \cos(0) + e^1 \cos(+1)\right]$$

$$= 1.88915335$$

$$= I_{approx_1}$$

$$|I_{approx_1} - I_{exact}| = 0.044268$$

$$= 4.4268 \times 10^{-2}$$

$$\langle p_n, p_m \rangle = \int_{-1}^{1} p_n(x)\, p_m(x)\, dx$$

$[-1, 1]$ Legendre Polynomials

$$\int_{-1}^{1} p_n(x)\, p_m(x) = 0$$

↳ Sequence of orthogonal $(m \neq n)$ polynomials $\{P_0(x), P_1(x), \ldots P_n(x), \ldots\}$

with the following properties

→ $P_n(1) = 1$ (monic polyn)

→ $\int_{-1}^{1} p(x)\, p_n(x) = 0$ for poly p of degree $< n$

$n \geq 2$ → $P_n(x) = \left(\frac{2n-1}{n}\right) x P_{n-1}(x) - \left(\frac{n-1}{n}\right) P_{n-2}(x)$

→ Roots (zeroes) of Legendre polynomials lie in $(-1, 1)$ & they are distinct.

→ These roots lie symmetrically on both the sides of origin (0).

Legendre polynomials

$$P_0(x) = 1 \qquad P_1(x) = x$$

$$P_2(x) = \frac{3}{2} x \times P_1(x) - \frac{1}{2} P_0(x)$$

$$= \frac{3}{2} x^2 - \frac{1}{2}$$

$$P_3(x) = \frac{5}{3} x P_2(x) - \frac{2}{3} P_1(x)$$

$$= \frac{5}{3} x \left(\frac{3}{2} x^2 - \frac{1}{2}\right) - \frac{2}{3} \times x$$

$$= \frac{5}{2} x^3 - \frac{5}{6} x - \frac{2}{3} x$$

$$P_3(x) = \frac{5}{2} x^3 - \frac{3}{2} x$$

→ nodes

TABLE 6.1 Gaussian Quadrature Nodes and Weights

$n+1$

n	Nodes x_i		Weights A_i	
1	$-\sqrt{\frac{1}{3}}$	x_0	1	A_0
	$+\sqrt{\frac{1}{3}}$	x_1	1	A_1
2	$-\sqrt{\frac{3}{5}}$	x_0	$\frac{5}{9}$	A_0
	0	x_1	$\frac{8}{9}$	A_1
	$+\sqrt{\frac{3}{5}}$	x_2	$\frac{5}{9}$	A_2
3	$-\sqrt{\frac{1}{7}(3-4\sqrt{0.3})}$	x_0	$\frac{1}{2}+\frac{1}{12}\sqrt{\frac{10}{3}}$	A_0
	$-\sqrt{\frac{1}{7}(3+4\sqrt{0.3})}$	x_1	$\frac{1}{2}-\frac{1}{12}\sqrt{\frac{10}{3}}$	A_1
	$+\sqrt{\frac{1}{7}(3-4\sqrt{0.3})}$	x_2	$\frac{1}{2}+\frac{1}{12}\sqrt{\frac{10}{3}}$	A_2
	$+\sqrt{\frac{1}{7}(3+4\sqrt{0.3})}$	x_3	$\frac{1}{2}-\frac{1}{12}\sqrt{\frac{10}{3}}$	A_3
4	$-\sqrt{\frac{1}{9}\left(5-2\sqrt{\frac{10}{7}}\right)}$		$0.3\left(\frac{-0.7+5\sqrt{0.7}}{-2+5\sqrt{0.7}}\right)$	
	$-\sqrt{\frac{1}{9}\left(5+2\sqrt{\frac{10}{7}}\right)}$		$0.3\left(\frac{0.7+5\sqrt{0.7})}{2+5\sqrt{0.7}}\right)$	
	0		$\frac{128}{225}$	
	$+\sqrt{\frac{1}{9}\left(5-2\sqrt{\frac{10}{7}}\right)}$		$0.3\left(\frac{-0.7+5\sqrt{0.7}}{-2+5\sqrt{0.7}}\right)$	
	$+\sqrt{\frac{1}{9}\left(5+2\sqrt{\frac{10}{7}}\right)}$		$0.3\left(\frac{0.7+5\sqrt{0.7}}{2+5\sqrt{0.7}}\right)$	

$P_2 \rightarrow$

$P_3 \rightarrow$

$P_4 \rightarrow$

$P_5 \rightarrow$

$$\sum_{i=0}^{n} A_i f(x_i)$$

x_i's are zeroes of Legendre poly

Legendre polynomials $[-1, 1]$

$$\int_a^b f(x)\,dx = \qquad (1)$$

$x \in [a, b] \qquad t \in [-1, 1]$

$$x = \frac{1}{2}\left[(b-a)t + (a+b)\right]$$

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

$$t = \frac{2x - a - b}{b-a}$$

If $x = a$
$\Rightarrow t = -1$

If $x = b$
$\Rightarrow t = +1$

$$\int_a^b f(x)\,dx = \int_{-1}^{1} f\left(\frac{1}{2}\left[(b-a)t + (a+b)\right]\right) \frac{b-a}{2}\,dt$$

$$= \frac{b-a}{2}\int_{-1}^{1} g(t)\,dt \qquad (2)$$

$$t = \frac{2x - a - b}{b-a}$$

Eg. $$\int_1^3 \{\underbrace{x^6 - x^2 \sin(2x)}_{f(x)}\}\,dx \approx 317.3442466$$

Trapezoidal method $h = 2$

$$\int_1^3 f(x)\,dx \approx \frac{h}{2}\left[f(a) + f(b)\right]$$

$$= \frac{2}{2}\left[f(1) + f(3)\right] = 731.6054420$$

Gauss-Legendre quadrature ($n = 1$ ie P_2 is used)

$t_0 = \frac{-1}{\sqrt{3}}$ $\quad t_1 = \frac{+1}{\sqrt{3}}$ $\quad A_0 = A_1 = 1$

$$\int_1^3 f(x)\,dx = \frac{2}{2}\int_{-1}^{1} f\Big[\underbrace{\tfrac{1}{2}(2t+4)}_{x=(t+2)}\Big]\,dt = \int_{-1}^{1} f(t+2)\,dt$$

$$= \int_{-1}^{1}\{\underbrace{(t+2)^6 - (t+2)^2 \sin(2t+4)}_{g(t)}\}\,dt$$

$$= 1 \times g(-1/\sqrt{3}) + 1\, g(1/\sqrt{3})$$

$$= \underline{\underline{306.81993}}$$ ✓

$[1, 3] = [1,2] \cup [2,3]$

$h = 1$

HW. Compare Simpson's $1/3$rd rule (x_0, x_1, x_2) of Gauss-Legendre quadrature with P_3.

Simpson's 333.2380940

Gauss-Leg 317.2641516

Eg. $\displaystyle\int_0^1 \frac{\sin x}{x}\, dx$

$\displaystyle\lim_{x \to 0} \frac{\sin x}{x} = 1$

$\hookrightarrow$ We cannot directly apply Simpson's $1/3$rd rule as it requires evaluating $\frac{\sin(0)}{0}$ which is undefined.

Gauss-Legendre

$$\int_0^1 \underbrace{\frac{\sin x}{x}}_{f}\, dx = \int_{-1}^{1} \frac{\sin\left(\frac{t+1}{2}\right)}{\left(\frac{t+1}{2}\right)} \frac{1}{2}\, dt$$

$[0,1] \to [-1,1]$

$t = 2x - 1$

$dt = 2dx$

$$= \frac{1}{2}\int_{-1}^{1} \frac{\sin\left(\frac{t+1}{2}\right)}{\left(\frac{t+1}{2}\right)}\, dt = \frac{1}{2}\int_{-1}^{1} f\left(\frac{t+1}{2}\right) dt$$

3

$$f(x) = \frac{\sin x}{x}$$

$n=1$ (using P_2)

$$t_0 = -\frac{1}{\sqrt{3}} \quad t_1 = \frac{1}{\sqrt{3}}$$

$$A_0 = 1 \quad A_1 = 1$$

$$\int_0^1 f(x)\,dx = \frac{1}{2}\int_{-1}^{1} f\left(\frac{t+1}{2}\right)dt \approx \frac{1}{2}\left[f\left(\frac{-1/\sqrt{3}+1}{2}\right) + f\left(\frac{1/\sqrt{3}+1}{2}\right)\right]$$

$$\approx 0.946041$$

$n=2$ (using P_3)

$$t_0 = -\sqrt{3/5} \quad t_1 = 0 \quad t_2 = +\sqrt{3/5}$$

$$A_0 = 5/9 \quad A_1 = 8/9 \quad A_2 = 5/9$$

$$\int_0^1 f(x)\,dx = \frac{1}{2}\int_{-1}^{1} f\left(\frac{t+1}{2}\right)dt$$

$$= \frac{1}{2} \times \frac{1}{9}\left[5 f\left(\overset{?}{\frac{-\sqrt{3/5}+1}{2}}\right) + 8 f\left(\overset{?}{\frac{0+1}{2}}\right) + 5 f\left(\overset{?}{\frac{\sqrt{3/5}+1}{2}}\right)\right]$$

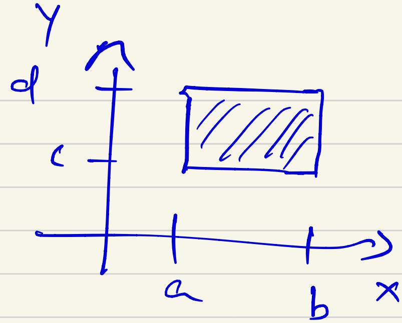
$$= 0.946083$$

$$\int_0^1 \frac{\sin x}{x}\,dx \approx 0.946083703$$

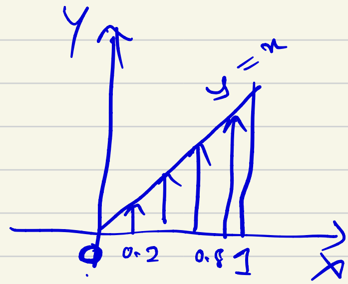
(MATLAB → Integral)

↳ In-built

$$\int_a^b \int_c^d f(x,y)\,dx\,dy$$

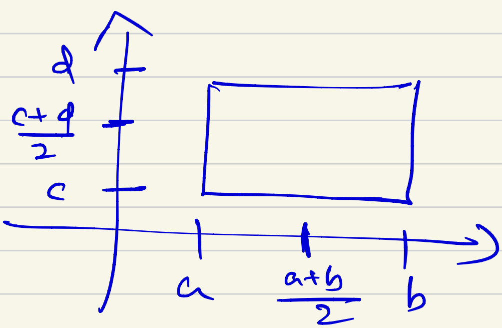


$$\int_0^1 \int_0^x f(x,y)\,dy\,dx$$



→ $x = 0$ to 1

$y = 0$ to x

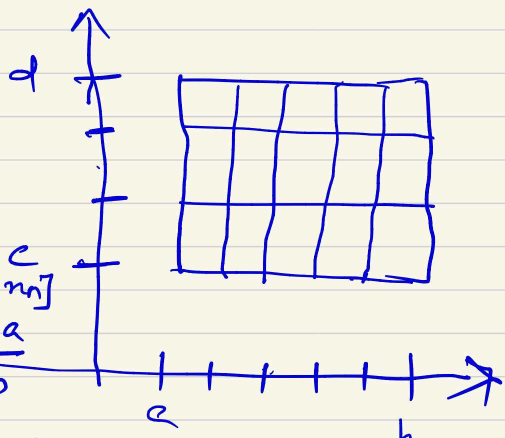


I Integration over a rectangular region

$$\iint_R f(x,y)\, dA \qquad R = \left\{ (x,y) \,\middle|\, \begin{matrix} a \le x \le b \\ c \le y \le d \end{matrix} \right\}$$

$$= [a,b] \times [c,d]$$

$$= \int_a^b \int_c^d f(x,y)\, dy\, dx = \int_c^d \int_a^b f(x,y)\, dx\, dy$$



Trapezoidal Rule

Divide $[a,b]$ into 'n' subintervals

$x_0 = a,$ $[x_0, x_1]\ [x_1, x_2]\ \cdots\ [x_{n-1}, x_n]$
$x_n = b$

$$x_i - x_{i-1} = h = \frac{b-a}{n}$$

Divide $[c,d]$ into 'm' subintervals

$y_0 = c$ $[y_0, y_1]\ [y_1, y_2]\ \cdots\ [y_{m-1}, y_m]$
$y_m = d$

$$y_j - y_{j-1} = k = \frac{d-c}{m}$$

$$\int_a^b \underbrace{\left(\int_c^d f(x,y)\, dy \right)}\, dx = \int_a^b g(x)\, dx$$

$$= \frac{h}{2} \left[g(x_0) + 2 \sum_{i=1}^{n-1} g(x_i) + g(x_n) \right] \quad (1)$$

$$f(x_i, y_j) = f_{ij}$$

$i = 0, 1, \ldots n$

$$g(x_i) = \int_c^d f(x_i, y)\, dy$$

$$= \frac{k}{2}\left[f(x_i, y_0) + 2\sum_{j=1}^{m-1} f(x_i, y_j) + f(x_i, y_m) \right] \quad 2$$

Use 2 for $g(x_0)$, $g(x_i)$ & $g(x_n)$ in 1

$$\int_a^b \int_c^d f(x,y)\, dy\, dx = \frac{hk}{4}\Bigg[\left(f_{00} + 2\sum_{j=1}^{m-1} f_{0j} + f_{0m}\right)$$

$$+ 2\sum_{i=1}^{n-1}\left(f_{i0} + 2\sum_{j=1}^{m-1} f_{ij} + f_{im}\right)$$

$$+ \left(f_{n0} + 2\sum_{j=1}^{m-1} f_{nj} + f_{nm}\right)\Bigg]$$

$$= \frac{hk}{4}\Bigg[\{f_{00} + f_{0m} + f_{n0} + f_{nm}\} + 4\sum_{i=1}^{n-1}\sum_{j=1}^{m-1} f_{ij}$$

$$+ 2\left\{\sum_{j=1}^{m-1}\left(f_{0j} + f_{nj}\right) + \sum_{i=1}^{n-1}\left(f_{i0} + f_{im}\right)\right\}\Bigg] \quad 3$$

Simpson's Rule ($1/3$ rd) (m & n $\rightarrow$ even)

$$\int_a^b \left(\int_c^d f(x,y)\, dy \right) dx = \int_a^b g(x)\, dx$$

$$= \frac{h}{3} \left[g(x_0) + 4 \sum_{i=1}^{n/2} g(x_{2i-1}) + 2 \sum_{i=1}^{n/2-1} g(x_{2i}) + g(x_n) \right] \rightarrow (4)$$

$$g(x_i) = \int_c^d f(x_i, y)\, dy$$

$$= \frac{k}{3} \left[f_{i,0} + 4 \sum_{j=1}^{m/2} f_{i,2j-1} + 2 \sum_{j=1}^{m/2-1} f_{i,2j} + f_{i,m} \right] \rightarrow (5)$$

Use (5) in (4)

$$\int_a^b \int_c^d f(x,y)\, dy\, dx \approx \frac{hk}{9} \Big[\{ f_{0,0} + f_{n,0} + f_{0,m} + f_{n,m} \} + 16 \left(\sum_{j=1}^{m/2} \sum_{i=1}^{n/2} f_{2i-1,2j-1} \right) + 8 \Big\{ \sum_{j=1}^{m/2} \sum_{i=1}^{n/2-1} f_{2i,2j-1} + \sum_{j=1}^{m/2-1} \sum_{i=1}^{n/2} f_{2i-1,2j} \Big\}$$

$$+4\left\{\sum_{i=1}^{n/2}\left(f_{2i-1,0}+f_{2i-1,m}\right)+\sum_{j=1}^{m/2}\left(f_{0,2j-1}+f_{n,2j-1}\right)+\sum_{j=1}^{m/2-1}\sum_{i=1}^{n/2-1}f_{2i,2j}\right\}$$

$$+\,2\left\{\sum_{i=1}^{n/2-1}\left(f_{2i,0}+f_{2i,m}\right)+\sum_{j=1}^{m/2-1}\left(f_{0,2j}+f_{n,2j}\right)\right\}\Bigg]$$

$$6$$

Curse of dimensionality.

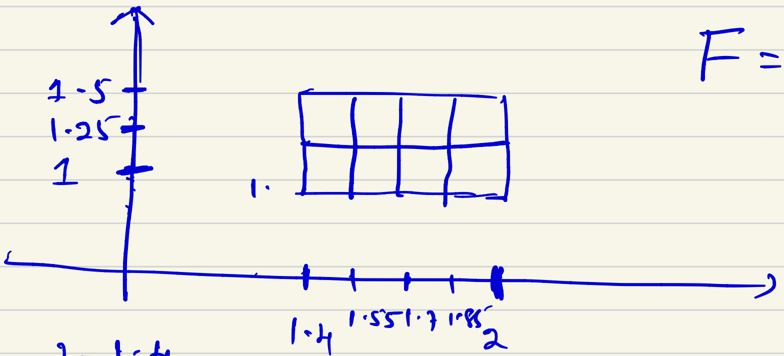
$$O(h^2+k^2)$$

$$O(h^4+k^4)$$

Eg: Use Trapezoidal & Simpson's (1/3rd) rule to evaluate

$$\int_{1.4}^{2} \int_{1}^{1.5} \log(x+2y)\, dy\, dx$$

with $h = 0.15$ $k = 0.25$



$F = (f_{ij})_{(n+1)(\times m+1)}$

$n = \dfrac{2-1.4}{0.15} = 4$ $x_0 = 1.4$ $x_1 = 1.55$

$x_2 = 1.7$ $x_3 = 1.85$ $x_4 = 2.$

$m = \dfrac{1.5-1}{0.25} = 2$ $y_0 = 1,\ y_1 = 1.25,\ y_2 = 1.5$

Trapezoidal

$$\frac{0.15}{2}\left[g(x_0) + 2\{g(x_1) + g(x_2) + g(x_3)\} + g(x_4)\right] \text{ --- } (1)$$

$$g(x_i) = \int_{1}^{1.5} \underbrace{\log(x_i + 2y)}_{f(x_i,y)}\, dy$$

$$= \frac{k}{2}\left[f_{i0} + 2 f_{i1} + f_{i2}\right] \text{ --- } (2)$$

$i = 0, 1, 2, 3, 4$

$$f(x,y) = \log(x+2y)$$

$x_0 = 1.4$ $\quad g(x_0) = g_0 = \frac{0.25}{2}\left[f_{00} + 2f_{01} + f_{02}\right]$

$=$

$x_1 = 1.55$ $\quad g(x_1) = \frac{0.25}{2}\left[f_{10} + 2f_{11} + f_{12}\right]$

$=$

$x_2 = 1.7$ $\quad g(x_2) = \frac{0.25}{2}\left[f_{20} + 2f_{21} + f_{22}\right]$

$x_3 = 1.85$ $\quad g(x_3) = \frac{0.25}{2}\left[f_{30} + 2f_{31} + f_{32}\right]$

$x_4 = 2$ $\quad g(x_4) = \frac{0.25}{2}\left[f_{40} + 2f_{41} + f_{42}\right]$

$=$

T.R ① $\Rightarrow$ 0.39623200 (verify)

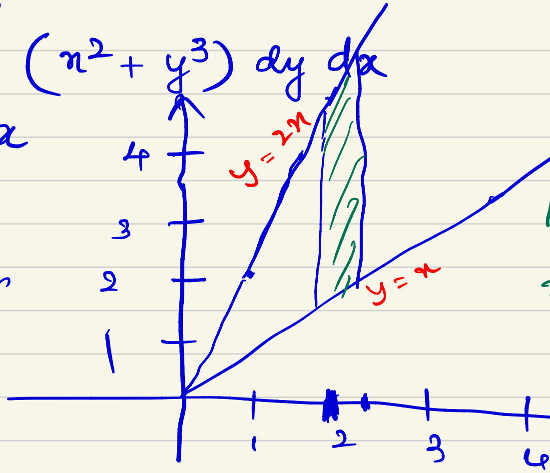
Simpson's 1/3rd rule: 0.429552438

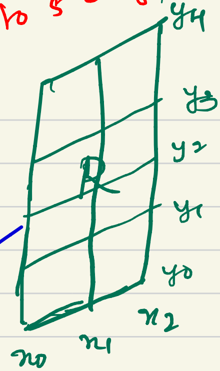
exact 0.4295545265

≈ 16.50864 (exact) upto 5 digits

Eg: $$\int_{2}^{2.2}\int_{x}^{2x}(x^2+y^3)\,dy\,dx$$

For each x,
y varies from x to $2x$





$n = 2$

$m = 4$

$h = 0.1$

$x_0 = 2$ $\qquad x_1 = 2.1$ $\qquad x_2 = 2.2$

$y = 2$ to 4 $\qquad k = \frac{4-2}{4} = 0.5$

$y_0 = 2$ $\quad y_1 = 2.5$ $\quad y_2 = 3$ $\quad y_3 = 3.5$ $\quad y_4 = 4$

$\underline{x_1 = 2.1}$ $\qquad y = 2.1$ to $2 \times 2.1 = 4.2$

$$k = \frac{4.2-2.1}{4} = 0.525$$

$y_0 = 2.1$ $\qquad y_1 = 2.625$ $\qquad y_2 = 3.15$

$y_3 = 3.675$ $\qquad y_4 = 4.2$

$\underline{x_2 = 2.2}$ $\qquad y = 2.2$ to 4.4 $\qquad k = \frac{4.4-2.2}{4} = 0.55$

$y_0 = 2.2$ $\qquad y_1 = 2.75$ $\qquad y_2 = 3.3$

$y_3 = 3.85$ $\qquad y_4 = 4.4$

$$\int_{2}^{2.2}\int_{x}^{2x} f(x,y)\,dy\,dx = \int_{2}^{2.2} g(x)\,dx$$

$$= \frac{0.1}{2}\left[\underline{g(2)} + 2\,\underline{g(2.1)} + \underline{g(2.2)}\right] \quad \text{—— } 1$$

$$f(x,y) = x^2 + y^3$$

$$g(2) = \int_{2}^{4} f(2,y)\,dy = \frac{0.5}{2}\Big[f(2,2) + 2\big(f(2,2.5) + f(2,3) + f(2,3.5)\big) + f(2,4)\Big]$$

$f(2,y) = 4 + y^3$

$$= 68.75$$

$$g(2.1) = \frac{0.525}{2}\Big[f(2.1,2.1) + 2\big(f(2.1,2.625) + f(2.1,3.15) + f(2.1,3.675)\big) + f(2.1,4.2)\Big]$$

$f(2.1,y) = 2.1^2 + y^3 = 4.41 + y^3$

$$= \underline{82.242}$$

$$\underline{83.1030}$$

$$g(2.2) = \frac{0.55}{2}\Big[f(2.2,2.2) + 2\big(f(2.2,2.75) + f(2.2,3.3) + f(2.2,3.85)\big) + f(2.2,4.4)\Big]$$

$f(2.2,y) = 2.2^2 + y^3 = 4.84 + y^3$

$$= 97.7441$$

$$= 99.5921$$

$1 \Longrightarrow 16.7274$

(16.5489)

HW Solve the same eq using Gauss-Legendre quadrature with $\begin{cases} n=1 & (\text{use } P_{n+1} = P_2) \\ n=2 & (\text{use } P_{n+1} = P_3) \end{cases}$

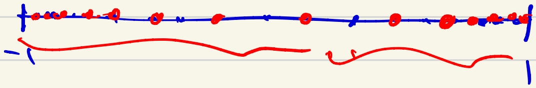
$\to$ Double integral variable limit

$\to$ $[-1, 1] \to$

Adaptive Simpson's 1/3rd rule

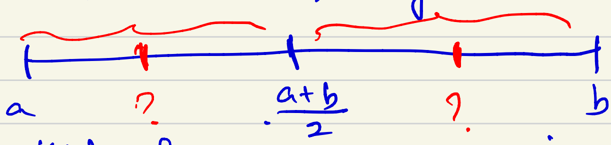
Trapezoidal & Simpson's rules
$\longrightarrow$ uniform node distribution
$h \to$ step size

Legendre quadrature



Consider $\int_a^b f(x)\,dx$ ———— (1)

Assume we want to approximate (1) within a specified tolerance, say $\epsilon > 0$

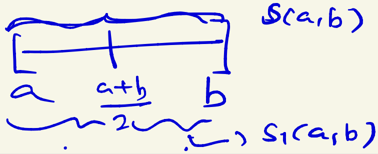


$$h = \frac{b-a}{2}$$

Simpson's 1/3rd rule

$$\int_a^b f(x)\,dx = \overbrace{\frac{h}{3}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]}^{S(a,b)} - \frac{h^5}{90} f^{(4)}(\xi_1)$$

$\boxed{\xi = \xi_1 = \xi_2}$



$$\frac{h^5}{90} f^{(4)}(\xi)$$

$$\int_a^b f(x)\,dx = S(a,b) - \frac{h^5}{90} f^{(4)}(\xi_1) \quad \text{--- (2)}$$

$a < \xi_1 < b$

$$S(a,b) = \frac{h}{2}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]$$

Choose $n = 4$ $\quad \frac{b-a}{4} = \frac{h}{2}$

$$\int_a^b f(x)\,dx = \underbrace{\frac{h/2}{3}\Big[\{f(a) + 4f(a+h/2) + f(a+h)\} + \{f(a+h) + 4f(a+\tfrac{3h}{2}) + f(b)\}\Big]}_{S_1(a,b)}$$

$$- \left(\frac{h}{2}\right)^4 \frac{b-a}{180} f^{(4)}(\xi_2) \quad \text{--- (3)}$$

$\frac{b-a}{2} \times 2$

a

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

a to $\frac{a+b}{2}$: $\quad \frac{h}{6}\left[f(a) + 4f(a+h/2) + f(a+h)\right] = S\left(a, \frac{a+b}{2}\right)$

$\frac{a+b}{2}$ to b: $\quad \frac{h}{6}\left[f(a+h) + 4f(a+\tfrac{3h}{2}) + f(b)\right] = S\left(\frac{a+b}{2}, b\right)$

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

$$(3) \Rightarrow \int_a^b f(x)\,dx = S\left(a, \frac{a+b}{2}\right) + S\left(\frac{a+b}{2}, b\right) - \frac{h^5}{16 \times 90} f^{(4)}(\xi_2)$$

ξ

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

Assume $f^{(4)}(x)$ does not vary much in $[a,b]$ $\quad$ (4)

$$f^{(4)}(\xi_1) \approx f^{(4)}(\xi_2)$$

Compare (2) & (4) (with $\xi_1 = \xi_2 = \xi$)

$$\int_a^b f(x)\,dx = S\left(a, \frac{a+b}{2}\right) + S\left(\frac{a+b}{2}, b\right) - \frac{1}{16}\left(\frac{h^5}{90}\right) f^{(4)}(\xi)$$

$$\approx S(a,b) - \frac{h^5}{90} f^{(4)}(\xi)$$

$$\frac{15}{16}\,\frac{h^5}{90} f^{(4)}(\xi) \approx \left[S(a,b) - \underbrace{\left\{ S\left(a, \frac{a+b}{2}\right) + S\left(\frac{a+b}{2}, b\right) \right\}}_{S_1(a,b)} \right]$$

<u>Error</u> $\dfrac{h^5}{90} f^{(4)}(\xi) \approx \dfrac{16}{15}\left[S(a,b) - \overbrace{S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right)}^{S_1(a,b)} \right]$ — (5)

Consider (4)

$$15\left| \int_a^b f(x)\,dx - \overbrace{\left\{ S\left(a, \frac{a+b}{2}\right) + S\left(\frac{a+b}{2}, b\right) \right\}}^{S_1(a,b)} \right|$$

$$\approx \frac{1}{16}\left(\frac{h^5}{90}\right) f^{(4)}(\xi)$$

$$\approx \frac{1}{\cancel{16}} \times \frac{\cancel{16}}{15}\left[S(a,b) - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right) \right]$$

15 actual error in 2nd formula (Simpson's 1/3) = error b/n 1st & 2nd Simpsons 1/3rd rules

$S_1(a,b)$ $\quad \frac{b-a}{4} = h/2$

i.e., $S\left(a, \frac{a+b}{2}\right) + S\left(\frac{a+b}{2}, b\right)$ approximates

$\int_a^b f(x)\,dx$ about 15 times better than

its agreement with $S(a,b)$ $\quad h = \frac{b-a}{2}$

$\xi_{\varphi_1} \approx \xi_{\varphi_2} = \xi_\varphi$

$$\left| \int_a^b f(x)\,dx - S_1(a,b) \right| \approx \frac{1}{16}\left(\frac{h^5}{90} f^{(4)}(\xi_\varphi)\right)$$

$$\left| S(a,b) - S_1(a,b) \right| \approx \frac{15}{16}\left(\frac{h^5}{90} f^{(4)}(\xi_\varphi)\right)$$

$$15 \left| \int_a^b f(x)\,dx - S_1(a,b) \right| \approx \left| S(a,b) - S_1(a,b) \right|$$

Monday 18/3/24
Quiz 8 – 8:50
15 weightage
+

Adaptive Simpson's 1/3rd rule

$$\int_0^{\pi/2} \sin x \, dx = 1$$

Compare $\frac{1}{15}\left| S(0,\pi/2) - \{S(0,\pi/4) + S(\pi/4,\pi/2)\}\right|$

with $\left| \underbrace{\int_0^{\pi/2} \sin x \, dx}_{1} - \{S(0,\pi/4) + S(\pi/4,\pi/2)\}\right|$

$h = \frac{b-a}{2} = \frac{\pi/2 - 0}{2} = \pi/4$

$$S(0,\pi/2) = \frac{\pi/4}{3}\left[f(0) + 4 f(\overbrace{0+h}^{\pi/4}) + f(\pi/2)\right]$$

$$= \frac{\pi}{12}\left[0 + 4 \times \frac{1}{\sqrt{2}} + 1\right] = \frac{\pi}{12}(1+2\sqrt{2})$$

$$= 1.0022798 78$$

$\frac{\pi/2}{2} = \frac{\pi/4}{2}$ $\quad S_1(0,\pi/2) = \underbrace{S(0,\pi/4)} + \underbrace{S(\pi/4,\pi/2)}$

$$= \frac{\pi/8}{3}\left[f(0) + 4f(\pi/8) + f(\pi/4)\right]$$

$$+ \frac{\pi/8}{3}\left[f(\pi/4) + 4f\left(\frac{3\pi}{8}\right) + f(\pi/2)\right]$$

$$= \pi/24\left[0 + 4 \times \sin(\pi/8) + \sin(\pi/4)\right]$$

$$+ \pi/24\left[\sin(\pi/4) + 4\sin(3\pi/8) + \sin(\pi/2)\right]$$

$$= \underbrace{0.292932 6378}_{S(0,\pi/4)} + \underbrace{0.7072019 47}_{S(\pi/4,\pi/2)}$$

$$= 1.00013 4585 \longrightarrow S_1(0,\pi/2)$$

$$I = \int_0^{\pi/2} \sin x \, dx = 1 \qquad S(0,\pi/2) = 1.0022798785$$

$$S_1(0,\pi/2) = 1.000134585$$

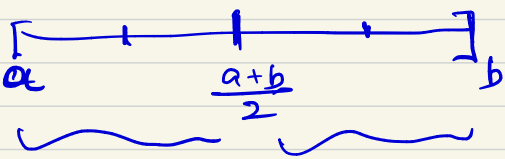
$$\left| I - S_1(0,\pi/2) \right| = 0.000134585 = 1.34585 \times 10^{-4}$$

$$\left| S(0,\pi/2) - S_1(0,\pi/2) \right| = 0.002145293$$

$$\frac{1}{15}\left| \quad " \quad \right| = \frac{1}{15} \times \; " = 0.000143020 = 1.43020 \times 10^{-4}$$

$\varepsilon = 10^{-6}$

$S(a,b)$ & $S_1(a,b)$ $\qquad S(a,b)$: $h = \frac{b-a}{2}$ $\qquad S_1(a,b)$: $h/2$



$\frac{a+b}{2} + \frac{b-a}{4}$

$h/2$ $\qquad S\left(a, \frac{a+b}{2}\right) \qquad S\left(\frac{a+b}{2}, b\right)$

$h/4 = \frac{b-a}{8}$

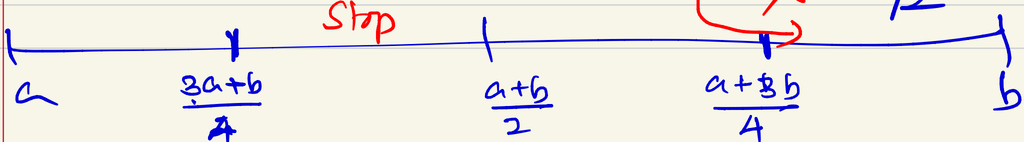
$$S_1\left(a, \frac{a+b}{2}\right) = S\left(a, \frac{3a+b}{4}\right) + S\left(\frac{3a+b}{4}, \frac{a+b}{2}\right)$$

$$S_1\left(\frac{a+b}{2}, b\right) = S\left(\frac{a+b}{2}, \frac{a+3b}{4}\right) + S\left(\frac{a+3b}{4}, b\right)$$

$$\frac{1}{15}\left| S\left(a, \frac{a+b}{2}\right) - S_1\left(a, \frac{a+b}{2}\right) \right| < \varepsilon/2$$

$$\frac{1}{15}\left| S\left(\frac{a+b}{2}, b\right) - S_1\left(\frac{a+b}{2}, b\right) \right| < \varepsilon/2$$

Stop



Method of undetermined coefficients

$$\int_a^b f(x)\,dx = w_1 f(a) + w_2 f\left(\frac{a+b}{2}\right) + w_3 f(b) \quad (1)$$

Find the weights such that the formula is exact for poly of degree ≤ 2

(formula has degree of precision 2)

$$\mathbb{P}_2 = \{ a_0 + a_1 x + a_2 x^2 \mid a_i \in \mathbb{R} \}$$

One Basis $\{1, x, x^2\}$

$f(x) = 1$

$$\int_a^b 1\,dx = w_1 \times 1 + w_2 \times 1 + w_3 \times 1$$

$$b - a = w_1 + w_2 + w_3 \quad (2)$$

$f(x) = x$

$$\int_a^b x\,dx = w_1 \times a + w_2 \left(\frac{a+b}{2}\right) + w_3 \times b$$

$$\frac{b^2 - a^2}{2} = w_1 a + w_2 \left(\frac{a+b}{2}\right) + w_3 b \quad (3)$$

$f(x) = x^2$

$$\int_a^b x^2\,dx = w_1 a^2 + w_2 \left(\frac{a+b}{2}\right)^2 + w_3 b^2$$

$$\frac{(b^3 - a^3)}{3} = w_1 a^2 + w_2 \left(\frac{a+b}{2}\right)^2 + w_3 b^2 \quad (4)$$

(2) – (4) lin sys for w_1, w_2 & w_3

$\xrightarrow{\text{Compute } w_i}$ Simpson's 1/3rd rule ?

Exc. Find the weights a, b, c, d so that the quadrature formula

$$\int_{-1}^{1} f(x)\,dx = a f(-1) + b f(1) + c f'(-1) + d f'(1)$$

exact for poly of degree ≤ 3 (degree of precision 3).