

## Numerical Methods

### Root Finding

$$\rightarrow \text{Regular Falsi} : x_{n+1} = b - f(b) \left( \frac{b-a}{f(b)-f(a)} \right)$$

$$\rightarrow \text{Secant} : x_{n+1} = x_n - f(x_n) \left( \frac{x_n - x_{n-1}}{f(x_n) - f(x_{n-1})} \right)$$

$$\rightarrow \text{Newton} : x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

$$\rightarrow \text{Modified Newton} : x_{n+1} = x_n - \frac{f(x_n) \cdot f'(x_n)}{(f'(x_n))^2 - f(x_n) \cdot f''(x_n)}$$

$\rightarrow$  Müller:

$$d_1 = \frac{f(x_1) - f(x_0)}{x_1 - x_0} \quad d_2 = \frac{f(x_2) - f(x_1)}{x_2 - x_1}$$

$$a = \frac{d_2 - d_1}{x_2 - x_0} \quad b = d_2 + a(x_2 - x_1) \quad (= f(x_n))$$

$$x_3 = x_2 - \frac{2c}{b + \text{sgn}(b) \sqrt{b^2 - 4ac}}$$

### Interpolation

$$\rightarrow \text{Lagrange Interpolation} : p(x) = \sum_{i=0}^n l_i(x) f(x_i), \quad l_i(x) = \prod_{j=0}^n \frac{x - x_j}{x_i - x_j}$$

$$\rightarrow \text{Newton's " : } p(x) = \sum_{k=0}^n f[x_0, \dots, x_k] \cdot \prod_{j=0}^{k-1} (x - x_j),$$

### Divided Difference

## System of Non-Linear Equations

$\rightarrow$  Fixed point method:

Rewrite eqns. as  $x_1 = g_1(\underline{x}) \dots x_n = g_n(\underline{x})$

$$\text{Necessary condn: } \left[ \left| \frac{\partial g_{ij}}{\partial x_i} \right| + \dots + \left| \frac{\partial g_{ij}}{\partial x_n} \right| \right] \leq 1, \forall 1 \leq j \leq n$$

→ Newton's method :  $\tilde{x}^{(i+1)} = \tilde{x}^{(i)} - J_{\tilde{x}^{(i)}}^{-1} \cdot f(\tilde{x}^{(i)})$ , where  $J_{\tilde{x}^{(i)}}$  is the Jacobian inverse evaluated at  $\tilde{x}^{(i)}$ .

### Least Squares for Functions

→ System of equations :  $\sum_{n=0}^N a_n \int_a^b x^{j+n} dx = \int_a^b x^j f(x) dx$

→ Orthogonal functions : (Alternative for least squares)

→ Weight function : An integrable function  $w$  is called a weight function on the interval  $I$  if  $w(x) > 0 \quad \forall x \in I$ .

→ Used to assign varying degrees of importance to approximations on certain portions of the interval.

→ Two functions are orthogonal w.r.t  $w$  if :

$$\int_a^b w(x) \phi_i(x) \phi_j(x) dx = \begin{cases} 0, & i \neq j \\ \omega_j > 0, & i = j \end{cases}$$

→ We can solve large least squares w/o matrix multiplication. We can reduce the system to:

$$a_i \int_a^b w(x) (f_i(x))^2 dx = \int_a^b w(x) y(x) f_i(x) dx, \quad i = 0, \dots, n$$

### Numerical Differentiation & Integration

→ Forward difference :  $f'_j = \frac{f_{j+1} - f_j}{h} + O(h)$

→ Backward " :  $f'_j = \frac{f_j - f_{j-1}}{h} + O(h)$

→ Central " :  $f'_j = \frac{f_{j+1} - f_{j-1}}{2h} + O(h^2)$

→ 3 point forward difference :  $f'_j \approx \frac{-3f_j + 4f_{j+1} - f_{j+2}}{2h}$

$$\rightarrow \text{"backward"} : f'_j \approx \frac{3f_j - 4f_{j-1} + f_{j-2}}{2h}$$

$$\rightarrow \text{Second derivative} : f''_j = \frac{f_{j+2} - 2f_{j+1} + f_j}{h^2} + O(h)$$

$\rightarrow$  Newton-Cotes formulae: Use equally spaced nodes

$\rightarrow$  Open: exclude end points  $\rightarrow$  Closed: include endpoints

$$\rightarrow \text{Trapezoidal Rule: } \int_a^b f(x) dx \approx \frac{h}{2} (f(a) + f(b)) - \frac{h^3}{12} f''(\xi)$$

$$\rightarrow \text{Simpson's } \frac{1}{3} \text{ Rule: } \int_{x_0}^{x_2} f(x) dx \approx \frac{h}{3} (f_0 + 4f_1 + f_2) - \frac{h^5}{90} f^{(4)}(\xi)$$

$$\rightarrow \text{Simpson's } \frac{3}{8} \text{ Rule: } \int_{x_0}^{x_3} f(x) dx \approx \frac{3h}{8} (f_0 + 3f_1 + 3f_2 + f_3) - \frac{3h^5}{80} f^{(4)}(\xi)$$

$$\rightarrow \text{Boole's Rule: } \int_{x_0}^{x_4} f(x) dx \approx \frac{2h}{45} (7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4) + \frac{8h^7}{945} f^{(6)}(\xi)$$

$\rightarrow$  Open formulae:

$$\rightarrow \text{Midpoint rule: } \int_{x_0}^{x_1} f(x) dx = h f_0 + \frac{h^3}{3} f''(\xi)$$

$$\rightarrow \text{Two-point open rule: } \int_{x_0}^{x_2} f(x) dx = \frac{3h}{2} (f_0 + f_1) + \frac{3h^3}{4} f''(\xi)$$

$$\rightarrow \text{Three-point open rule: } \int_{x_0}^{x_3} f(x) dx = \frac{4h}{3} (2f_0 + f_1 + 2f_2) + \frac{14h^5}{45} f^{(4)}(\xi)$$

$$\rightarrow \text{Four-point open rule: } \int_{x_0}^{x_4} f(x) dx = \frac{5h}{24} (11f_0 + f_1 + f_2 + 11f_3) + \frac{95h^5}{144} f^{(4)}(\xi)$$

$$\rightarrow \text{Composite Trapezoidal} = \int_a^b f(x) dx = \frac{h}{2} \left( f(a) + 2 \sum_{j=1}^{n-1} f(x_j) + f(b) \right) + \frac{b-a}{12} h^2 f''(g)$$

$\rightarrow$  Composite Simpsons:

$$\int_a^b f(x) dx = \frac{h}{3} \left( f(a) + 2 \sum_{j=1}^{\frac{n}{2}-1} f(x_{2j}) + 4 \sum_{j=1}^{\frac{n}{2}} f(x_{2j+1}) + f(b) \right) + \frac{b-a}{180} h^4 f^{(4)}(g)$$

$\rightarrow$  Richardson's Extrapolation

let  $I_{\text{true}} = \int_a^b f(x) dx$ ,  $I(h)$  be trapezium rule with  $h$  as length of interval, and  $E(h)$  be error when using trapezium rule

$$\text{we know: } I(h) + E(h) = I(\frac{h}{2}) + E(\frac{h}{2}) = I_{\text{true}}$$

$$\text{let us take } c = -\frac{f''(n)}{12}$$

$$I_{\text{true}} = I(h) + ch^3 \quad \textcircled{1}$$

$$\begin{aligned} I_{\text{true}} &= I(\frac{h}{2}) + 2c(\frac{h}{2})^3 \\ &= I(\frac{h}{2}) + \frac{ch^3}{2^2} \quad \textcircled{2} \end{aligned}$$

$$-1 \times \textcircled{1} + 4 \times \textcircled{2}$$

$$\Rightarrow -I(h) - ch^3 + 4I(\frac{h}{2}) + ch^3 = -I_{\text{true}} + 4I_{\text{true}}$$

$$I_{\text{true}} = \frac{4I(\frac{h}{2}) - I(h)}{3} \quad \left. \right\} \text{Richardson's extrapolation}$$

$$\text{Final: } I_{\text{true}} = \frac{2^{n-1} I(\frac{h}{2}) - I(h)}{2^{n-1} - 1} + \frac{ch^{n+1}}{2^{n+2} - 2} \quad \text{error}$$

→ Increases level of accuracy by 1.

→ Romberg Integration

→ Use Richardson's extrapolation multiple times

$$\text{I.e } I(h, h_{1/2}) = I(h_{1/2}) + \frac{I(h_{1/2}) - I(h)}{3}$$

$$I(h_{1/2}, h_{1/4}) = I(h_{1/4}) + \frac{I(h_{1/4}) - I(h_{1/2})}{3}$$

$$I(h, h_{1/2}, h_{1/4}) = I(h_{1/2}, h_{1/4}) - I(h, h_{1/2})$$

⋮  
Eventually,  $I(h, \dots, h_{2^n})$  will get more accurate.

→ Method of undetermined coefficients:

$$\text{Let } I_{\text{Trapezoid}} = a_1 f(a) + a_2 f(b)$$

$$\text{if } f(x) = 1, \quad I_{\text{Trapezoid}} = a_1 + a_2 = \int_a^b 1 dx = b-a \quad ①$$

$$\cdot f(x) = x, \quad I_{\text{Trapezoid}} = a_1 \cdot a + a_2 \cdot b = \int_a^b x dx = \frac{b^2 - a^2}{2} \quad ②$$

$$-a \times ① + ② \Rightarrow \cancel{-a a_1 - a a_2 + a a_1 + b a_2} = a^2 - ab + \frac{b^2 - a^2}{2}$$
$$\cancel{b a_2 - a a_2} = \frac{b^2 - 2ab + a^2}{2}$$

$$\cancel{(b-a) a_2} = \frac{(b-a)^2}{2}$$

$$\therefore a_2 = \frac{b-a}{2}, \quad a_1 = b-a - \frac{b-a}{2} = \frac{b-a}{2}$$

$$\therefore I_{\text{Trapezoid}} = a_1 f(a) + a_2 f(b) = \frac{b-a}{2} (f(a) + f(b))$$

(some us before)

→ Gaussian Quadrature

→ Rather than use points at equally spaced points, we choose the points in an optimal way.

→ Used to calculate:

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

any integral can be brought to this form

→ Applying method of undetermined coefficients (upto  $x^3$ , not  $x$ ), we get this to be the final result:

$$\int_{-1}^1 f(x) dx = f(-\sqrt{3}) + f(\sqrt{3})$$

### DDEs - IVPs

→ Peano existence theorem: (sufficient)

If  $f(x, y)$  is continuous in  $R = \{(x-x_0) \leq a, |y-y_0| \leq b\}$ , then IVP will have at least one soln. in the interval  $|x-x_0| \leq h$ , where:

$$h = \min \left\{ a, \frac{b}{M} \right\}, M = \max_{(x,y) \in R} \{f(x, y)\}$$

→ Picard's theorem: (sufficient)

If  $f(x, y) \& \frac{\partial f}{\partial y}$  are continuous in  $R = \{(x-x_0) \leq a, |y-y_0| \leq b\}$ ,

the IVP has a unique soln. in the interval  $|x-x_0| \leq h$ , where:

$$h = \min \left\{ a, \frac{b}{M} \right\}, M = \max_{(x,y) \in R} \{f(x, y)\}$$

→ Picard iteration:  $y_n(x) = y(x_0) + \int_{x_0}^x f(t, y_{n-1}(t)) dt$

→ Euler's Method:  $y_{n+1} = y_n + hf(x_n, y_n)$

→ When the function cannot be integrated, but is infinitely differentiable

→ Modified Euler (Predictor - Corrector) method:

→ Euler is not very accurate.

$$y_{n+1} = y_n + \frac{h}{2} [f(x_n, y_n) + f(x_{n+1}, y_n + hf(x_n, y_n))]$$

→ Lip-shit condition:

A function satisfies Lip-shit condn. in the variable  $y$  on  $R$  if a constant  $L \geq 0$ , exist s.t.

$$|f(x, y_1) - f(x, y_2)| \leq L |y_2 - y_1|$$

Lipshitz constant

→ RK methods

→ Taylor series method requires partial derivatives every time

→ RK-2:

$$y_{n+1} = y_n + \frac{1}{2}(k_1 + k_2), \text{ where } k_1 = hf(x_n, y_n)$$

$$k_2 = hf(x_n + h, y_n + k_1)$$

→ RK-4

$$y_{n+1} = y_n + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

$$\text{, where } k_1 = hf(x_n, y_n)$$

$$k_2 = hf\left(x_n + \frac{h}{2}, y_n + \frac{k_1}{2}\right)$$

$$k_3 = hf\left(x_n + \frac{h}{2}, y_n + \frac{k_2}{2}\right)$$

$$k_4 = hf(x_n + h, y_n + k_3)$$

→ Higher order differential eqns.:

$$y^{(m)}(x) = f(x, y, y', \dots, y^{(m-1)}), a \leq x \leq b$$

$$y(a) = \alpha_1, \dots, y^{(m-1)}(a) = \alpha_{m-1}$$

→ Single step methods

$$\rightarrow \text{Process: } y(x_{n+1}) = f(x_n, y_n, y'_n, h)$$

\* Process is demanding only one past value.

→ Taylor series method

Assumption: The differential eqn. has a unique soln., and continuous partial derivatives of order  $(p+1)$

$$\frac{dy}{dx} = f(x, y) \quad y(x_0) = y_0 \quad a \leq x \leq b$$

Differentiate:

$$\frac{d^2y}{dx^2} = \frac{\delta f}{\delta x} + \frac{\delta y}{\delta x} \cdot \frac{dy}{dx} \Rightarrow y'' = f_x + f_y f$$

Similarly, we can get  $y^{(3)}, y^{(4)} \dots$

Using Taylor series:

$$y(x_1) = \sum_{i=0}^{\infty} \frac{h^i}{i!} \cdot y^{(i)}(x_0)$$

→ Multistep method

$$\rightarrow \text{general form: } y_{j+1} = \sum_{n=1}^m a_n y_{j-n+1} + h \sum_{k=0}^m b_k f_{j-k+1}$$

→ " of Adams' multistep methods:

$$y_{j+1} = y_j + h \sum_{k=0}^m b_k f_{j-k+1}$$

→ Adams Bashforth technique (when  $b_0 = 0$ )

→ Because  $b_0 = 0$ , the method is explicit, i.e. does not require calculation of  $f_{j+1}$ .

→ E.g. for a 3-step Adams Bashforth method,

$$y_{j+1} = y_j + h(b_1 f_j + b_2 f_{j-1} + b_3 f_{j-2})$$

How do we get the  $b$ -values? Construct an interpolating polynomial for  $f$  on  $x_j, x_{j-1}, x_{j-2}$ , and integrate it.

$$\text{We get } b_1 = \frac{23}{12}, b_2 = -\frac{4}{3}, b_3 = \frac{5}{12}$$

$$\therefore y_{j+1} = y_j + h \left( \frac{23}{12} f_j - \frac{4}{3} f_{j-1} + \frac{5}{12} f_{j-2} \right)$$

\* Use Euler / RK methods to get initial values.

→ Adams Moulton technique ( $b_0 \neq 0 \Rightarrow \text{Implicit Method}$ )

→ Derive in a similar way as Adams Moulton method

## ODEs - BVP

→ Consider a BVP:  $y'' = f(x, y, y')$ ,  $a \leq x \leq b$ ,  $y(a) = \alpha$ ,  $y(b) = \beta$

→ Shooting method (reduce BVP to IVP)

→ Existence theorem:

If  $f, f_y, f_{yy}$  are continuous on  $a \leq x \leq b$ , and:

i)  $f_y(x, y, y') > 0$  in  $a \leq x \leq b$

ii)  $|f_{yy}(x, y, y')| \leq M$  in  $a \leq x \leq b$

→ Linear BVP:  $y'' = f(x, y, y')$

$$= p(x)y' + q(x)y + r(x)$$

→ If  $p, q, r$  are continuous, and  $q > 0$  on  $a \leq x \leq b$ ,  
then the BVP has a unique soln.

→ Split into two IVPs:

$$\textcircled{1} \quad y'' = p(x)y' + q(x)y + r(x), \quad y(a) = \alpha, \quad y'(a) = 0$$

$$\textcircled{2} \quad y'' = p(x)y' + q(x)y, \quad y(a) = 0, \quad y'(a) = 1$$

If  $\textcircled{1}$  has soln.  $y_1$  &  $\textcircled{2}$  has soln  $y_2$ ,

→ Finite-difference methods for linear problems:

→ Consider the 2nd order BVP:

$$y'' = p(x) \frac{dy}{dx} + q(x)y + r(x), \quad x \in [a, b], \quad y(a) = \alpha, \quad y(b) = \beta$$

If  $p(x), q(x), r(x)$  are continuous on  $[a, b]$ , and  $q(x) > 0$  on  $[a, b]$ , then the tridiagonal linear system has a unique

$$\text{soln if } h < \frac{2}{\max_{[a,b]} |p(x)|}$$

→ Finite difference methods for Non-linear problems

Consider the BVP:

$$y'' = f(x, y, y'), x \in [a, b], y(a) = \alpha, y(b) = \beta$$

- If:
- 1)  $f, f_y$  &  $f_{yy}$  are continuous on  $x \in [a, b]$
  - 2)  $f_y \geq \delta > 0$  on  $x \in [a, b]$
  - 3) There exist constants  $K & L$  s.t:

$$n = \max_{x \in [a, b]} |f_y| \quad \& \quad L = \max_{x \in [a, b]} |f_{yy}|$$

Then there exists a unique soln. to the BVP.

Divide the interval into  $(N+1)$  equal sub-intervals, and replace  $y''(x_i)$  &  $y'(x_i)$  with the central difference formulae:

$$y'' = f(x, y, y')$$

$$\frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} = f(x_i, y_i, \frac{y_{i+1} - y_{i-1}}{2h})$$

There will be a unique soln. if  $h < \frac{2L}{\delta}$

### PDEs

$$\text{Second order P.D.E: } A \frac{\partial^2 u}{\partial x^2} + B \frac{\partial^2 u}{\partial x \partial y} + C \frac{\partial^2 u}{\partial y^2} + D \frac{\partial u}{\partial x} + E \frac{\partial u}{\partial y} + F_u = 0$$

- $A, B, \dots, F$  can be functions of  $x, y$
- If  $B^2 - 4AC = 0$ , parabolic eqn.
- " "  $> 0$ , hyperbolic "
- " "  $< 0$ , elliptic "