Numerical Methods

Root Finding

→ Regula Falsi : $x_{n+1} = b - f(b)\left(\dfrac{b-a}{f(b)-f(a)}\right)$

→ Secant : $x_{n+1} = x_n - f(x_n)\left(\dfrac{x_n - x_{n-1}}{f(x_n) - f(x_{n-1})}\right)$

→ Newton : $x_{n+1} = x_n - \dfrac{f(x_n)}{f'(x_n)}$

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

→ Müller :

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

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

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

Interpolation

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

→ 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

→ Fixed point method :

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

Necessary condn: $\left[\left|\dfrac{\delta g_i}{\delta x_1}\right| + \dots + \left|\dfrac{\delta g_i}{\delta x_n}\right|\right] \le 1, \ \forall\, 1 \le j \le n$

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

Least Squares for functions

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

→ Orthogonal functions : (Alternative for least squares)

- → Weight function : An integrable function w is called a weight function on the interval I if $w(x) > 0 \ \forall\, x \in I$.
  - → Used to assign varying degrees of importance to approximations on certain portions of the interval.
- → Two functions are orthogonal w.r.t w if :

$$\int_a^b w(x)\, \phi_k(x)\, \phi_j(x)\, dx = \begin{cases} 0, & j \neq k \\ \alpha_j > 0, & j \neq k \end{cases}$$

- → 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 : $f_j' = \dfrac{f_{j+1} - f_j}{h} + O(h)$

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

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

→ 3-point forward difference : $f_j' \simeq \dfrac{-3f_j + 4f_{j+1} - f_{j+2}}{2h}$

→ " backward " : $f_j' \approx \frac{3f_j - 4f_{j-1} + 4_{j-2}}{2h}$

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

→ Newton-Cotes formulae : Use equally spaced nodes

→ Open : exclude end points → Closed : include endpoints

→ Trapezoidal Rule : $\int_a^b f(x)\,dx \approx \frac{h}{2}(f(a)+f(b)) - \frac{h^3}{12} f''(\xi)$
(n=1)

→ Simpsons ⅓ Rule : $\int_{x_0}^{x_2} f(x)\,dx \approx \frac{h}{3}(f_0 + 4f_1 + f_2) - \frac{h^5}{90} f^{(4)}(\xi)$
(n=2)

→ Simpsons 3/8 Rule = $\int_{x_0}^{x_3} f(x)\,dx \approx \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3) - \frac{3h^5}{80} f^{(4)}(\xi)$
(n=3)

→ Boole's Rule = $\int_{x_0}^{x_4} f(x)\,dx \approx \frac{2h}{45}(7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4) + \frac{8h^7}{945} f^{(6)}(\xi)$
(n=4)

→ Open formulae:

→ Midpoint rule : $\int_{x_0}^{x_1} f(x)\,dx = 2hf_0 + \frac{h^3}{3} f''(\xi)$
(n=0)

→ Two-point open rule : $\int_{x_0}^{x_2} f(x)\,dx = \frac{3h}{2}(f_0 + f_1) + \frac{3h^3}{4} f''(\xi)$
(n=1)

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

→ Four point open rule : $\int_{x_0}^{x_4} f(x)\,dx = \frac{5h}{24}(11f_0 + f_1 + f_2 + 11f_3) + \frac{95h^5}{144} f^{(4)}(\xi)$
(n=3)

→ Composite Trapezoidal : $\int_a^b f(x)\,dx = \frac{h}{2}\left(f(a) + 2\sum_{j=1}^{n-1} f(x_j) + f(b)\right)$

$+ \frac{b-a}{12} h^2 f''(\xi)$

→ Composite Simpsons:

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

$$+ \frac{b-a}{180} h^4 f^{(4)}(\xi)$$

→ Richardson's Extrapolation

Let $I_{true} = \int_a^b f(x)\,dx$, $I(h)$ be trapezium rule with h as length of interval, and

$E(h)$ be error when using trapezium rule

We know : $I(h) + E(h) = I(h/2) + E(h/2) = I_{true}$

Let us take $c = -\frac{f''(\mu)}{12}$

$I_{true} = I(h) + ch^3$ ①

$I_{true} = I(h/2) + 2c(h/2)^3$

$= I(h/2) + \frac{ch^3}{2^2}$ ②

$-1 \times ① + 4 \times ②$

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

$I_{true} = \frac{4I(h/2) - I(h)}{3}$ } Richardson's extrapolation

Final : $I_{true} = \frac{2^{n-1} I(h/2) - I(h)}{2^{n-1} - 1} + \frac{c_2 h^{n+1}}{2^{n+2} - 2}$ ← Error

→ Increases level of accuracy by 1.

→ Romberg Integration

→ Use Richardson's extrapolation multiple times

i.e $I(h, h/_2) = I(h/_2) + \frac{I(h/_2) - I(h)}{3}$

$I(h/_2, h/_4) = I(h/_4) + \frac{I(h/_4) - I(h/_2)}{3}$

$I(h, h/_2, h/_4) = I(h/_2, h/_4) - I(h, h/_2)$

$\vdots$

Eventually, $I(h, \ldots, h/_{2^n})$ will get more accurate.

→ Method of undetermined coefficients:

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

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

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

$-a \times ① + ② \Rightarrow \cancel{-aa_1} - aa_2 + \cancel{aa_1} + ba_2 = a^2 - ab + \frac{b^2-a^2}{2}$

$ba_2 - aa_2 = \frac{b^2 - 2ab + a^2}{2}$

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

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

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

(same as before)

→ Gaussian Quadrature

→ Rather than use points at equally spaced points, we choose the points in a 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:

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

ODEs - IVPs

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

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

→ Picard's theorem: (sufficient)
If $f(x,y)$ & $\frac{\delta f}{\delta y}$ 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:

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

→ 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.

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

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

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

Lipshit constant

→ RK methods

→ Taylor series method requires partial derivates every time

→ RK-2:

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

→ RK-4

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

, 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.:

$$y^{(m)}(x) = f(x, y, y', \ldots, y^{(m-1)}), \quad a \le x \le b$$
$$y(a) = \alpha_1, \ldots, y^{(m-1)}(a) = \alpha_{m-1}$$

→ Single step methods

→ 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 derivates of order $(p+1)$

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

Differentiate:

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

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

Using Taylor series:

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

→ Multistep method

→ General form: $y_{j+1} = \sum_{k=1}^{m} a_k y_{j-k+1} + h \sum_{k=0}^{m} b_k f_{j-k+1}$

→ " " of Adam's 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}.

→ Eg: for a 3-step Adam 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.

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

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

* Use Euler / RK methods to get initial values.

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

→ Derive in a similar way as Adams Moulton method

→ Common Adam-Bashforth & Adam-Moulton method values

Order	Adam-Bashforth	Adam-Moulton
2	$0, 3/2, -5/2$	$\frac{5}{2}, \frac{8}{2}, -\frac{1}{2}$
3	$0, \frac{23}{12}, -\frac{16}{12}, \frac{5}{12}$	$\frac{9}{24}, \frac{19}{24}, \frac{-5}{24}, \frac{1}{24}$
4	$0, \frac{55}{24}, -\frac{59}{24}, \frac{37}{24}, -\frac{9}{24}$	$\frac{251}{720}, \frac{646}{720}, -\frac{264}{720}, \frac{106}{720}, -\frac{19}{720}$
5	$0, \frac{1901}{720}, -\frac{2774}{720}, \frac{2616}{720}, -\frac{1274}{720}, \frac{251}{720}$	

ODEs - BVP

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

→ Shooting method (reduce BVP to IVP)

→ Existence theorem:

If f, f_y & $f_{y'}$ is continuous on $a \le x \le b$, and:

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

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

→ 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 $a \le x \le b$, then the BVP has a unique soln.

→ Split into two IVPs:

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

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

If ① has soln. y_1 & ② has soln y_2,

→ Finite-difference methods for linear problems:

→ Consider the 2nd order BVP:

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

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

→ Finite difference methods for Non-linear problems

Consider the BVP:

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

If: 1) f, f_y & $f_{y'}$ 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.:

$$K = \max_{x \in [a,b]} |f_y| \quad \& \quad L = \max_{x \in [a,b]} |f_{y'}|$$

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:

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

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

There will be a unique soln. if $h < 2/L$

PDEs

Second order P.D.E: $A\dfrac{\delta^2 u}{\delta x^2} + B\dfrac{\delta^2 u}{\delta x \delta y} + C\dfrac{\delta^2 u}{\delta y^2} + D\dfrac{\delta u}{\delta x} + E\dfrac{\delta u}{\delta y} + Fu = 0$

→ $A, B, \ldots, F$ can be functions of x, y

→ If $B^2 - 4AC = 0$, parabolic eqn.

→ " " > 0, hyperbolic "

→ " " < 0, elliptic "